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(FILE 'HOME' ENTERED AT 08:30:43 ON 01 NOV 2004)

[REDACTED] ENTERED AT 08:30:55 ON 01 NOV 2004

FILE 'REGISTRY' ENTERED AT 08:31:20 ON 01 NOV 2004

FILE 'HCAPLUS' ENTERED AT 08:31:23 ON 01 NOV 2004
L2 TRA L1 1- RN : 11 TERMS

[REDACTED] ENTERED AT 08:31:24 ON 01 NOV 2004

[REDACTED] ENTERED AT 08:31:37 ON 01 NOV 2004

=> b hcap

[REDACTED] ENTERED AT 08:32:06 ON 01 NOV 2004
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FILE COVERS 1907 - 1 Nov 2004 VOL 141 ISS 19
FILE LAST UPDATED: 31 Oct 2004 (20041031/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

[REDACTED]

L1 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:376823 HCAPLUS
DN 138:365147
ED Entered STN: 16 May 2003
TI Compositions, methods and kits pertaining to luminescent compounds
IN Wood, Keith; Hawkins, Erika; Scurria, Mike; Klaubert, Dieter
PA Promega Corporation, USA
SO PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D211-70
ICS C07D241-02; C07D413-00; C12N009-02; C12Q001-34; C12Q001-66;
G01N033-53
CC 9-14 (Biochemical Methods)
Section cross-reference(s): 80
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|--------------|
| PI WO 2003040100 | A1 | 20030515 | WO 2002-US34972 | 20021101 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 2003153090 | A1 | 20030814 | US 2001-53482 | 20011102 <-- |

EP 1451155 A1 20040901 EP 2002-802815 20021101
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
 PRAI US 2001-53482 A 20011102
 WO 2002-US34972 W 20021101

CLASS

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

 WO 2003040100 ICM C07D211-70
 ICS C07D241-02; C07D413-00; C12N009-02; C12Q001-34;
 C12Q001-66; G01N033-53

OS MARPAT 138:365147

AB A method of measuring the enzymic activity of a luciferase includes contacting a luminogenic protein, such as a luciferase, with a protected luminophore to form a composition; and detecting light produced from the composition. The protected luminophore provides increased stability and improved signal-to-background ratios relative to the corresponding unmodified coelenterazine.

ST compn kit pertaining luminescent compd protein

IT Cell

Luminescent substances
 (compns., methods and kits pertaining to luminescent compds.)

IT Proteins

RL: ARU (Analytical role, unclassified); ANST (Analytical study)
 (luminogenic; compns., methods and kits pertaining to luminescent compds.)

IT 61869-41-8, Renilla luciferase

RL: ARU (Analytical role, unclassified); ANST (Analytical study)
 (compns., methods and kits pertaining to luminescent compds.)

IT 50909-86-9P 55779-48-1P 65417-16-5P 70217-82-2P 524066-91-9P

524066-92-0P 524066-93-1P 524066-94-2P 524066-95-3P 524066-96-4P

RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST
 (Analytical study); PREP (Preparation)
 (compns., methods and kits pertaining to luminescent compds.)

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Bryan; US 6416960 B1 2002 HCPLUS
- (2) Garini; US 6165734 A 2000 HCPLUS
- (3) Hideshi, N; Journal American Chem Society 2001, V123, P1523
- (4) Inouye, S; Biochemical and Biophysical Research Communications 1997, V233, P349 HCPLUS
- (5) Jones, K; Trends in Biotechnology 1999, V17, P477 HCPLUS
- (6) Roelant; US 6171809 B1 2001 HCPLUS
- (7) Shimomura, O; Biochemistry Journal 1989, V261, P913 HCPLUS
- (8) Shimomura, O; Biochemistry Journal 1995, V306, P537 HCPLUS

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 provided by InfoChem.

STRUCTURE FILE UPDATES: 29 OCT 2004 HIGHEST RN 772333-32-1
 DICTIONARY FILE UPDATES: 29 OCT 2004 HIGHEST RN 772333-32-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

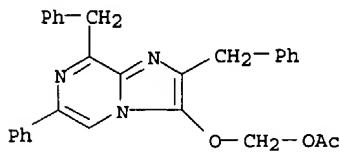
Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
 information enter HELP PROP at an arrow prompt in the file or refer
 to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

L3 ANSWER 1 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 524066-96-4 REGISTRY
 CN Methanol, [[6-phenyl-2,8-bis(phenylmethyl)imidazo[1,2-a]pyrazin-3-yl]oxy]-

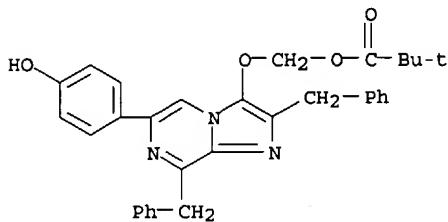
FS , acetate (ester) (9CI) (CA INDEX NAME)
 MF 3D CONCORD
 MF C29 H25 N3 O3
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL
 DT.CA Cplus document type: Patent
 RL.P Roles from patents: ANST (Analytical study); PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

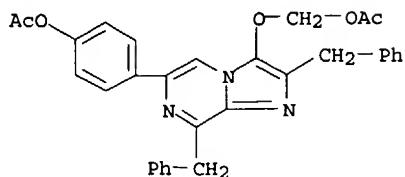
L3 ANSWER 2 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 524066-95-3 REGISTRY
 CN Propanoic acid, 2,2-dimethyl-, [{6-(4-hydroxyphenyl)-2,8-bis(phenylmethyl)imidazo[1,2-a]pyrazin-3-yl}oxy]methyl ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C32 H31 N3 O4
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL
 DT.CA Cplus document type: Conference; Patent
 RL.P Roles from patents: ANST (Analytical study); PREP (Preparation)
 RLD.NP Roles for non-specific derivatives from non-patents: BIOL (Biological study); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

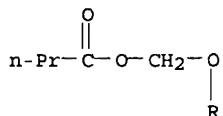
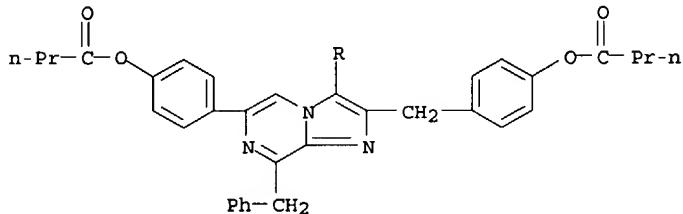
L3 ANSWER 3 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 524066-94-2 REGISTRY
 CN Phenol, 4-[(acetoxy)methoxy]-2,8-bis(phenylmethyl)imidazo[1,2-a]pyrazin-6-yl-, acetate (ester) (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C31 H27 N3 O5
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL
 DT.CA Cplus document type: Patent
 RL.P Roles from patents: ANST (Analytical study); PREP (Preparation)



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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

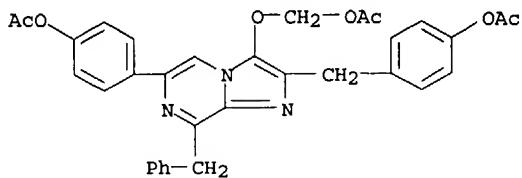
L3 ANSWER 4 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
RN 524066-93-1 REGISTRY
CN Butanoic acid, 4-[(1-oxobutoxy)methoxy]-2-[(4-(1-oxobutoxy)phenyl)methyl]imidazo[1,2-a]pyrazin-6-yl phenyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C39 H41 N3 O7
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: ANST (Analytical study); PREP (Preparation)



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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

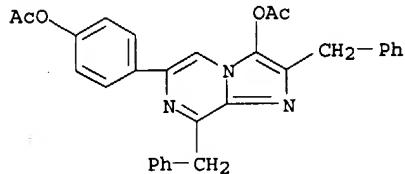
L3 ANSWER 5 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
RN 524066-92-0 REGISTRY
CN Phenol, 4-[(1-oxobutoxy)methoxy]-2-[(4-(1-oxobutoxy)phenyl)methyl]-8-(phenylmethyl)imidazo[1,2-a]pyrazin-6-yl-, acetate (ester) (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C33 H29 N3 O7
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: ANST (Analytical study); PREP (Preparation)



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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

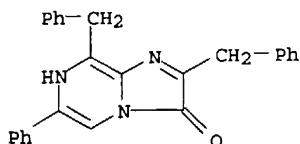
L3 ANSWER 6 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 524066-91-9 REGISTRY
 CN Imidazo[1,2-a]pyrazin-3-ol, 6-[4-(acetoxy)phenyl]-2,8-bis(phenylmethyl)-, acetate (ester) (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C30 H25 N3 O4
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL
 DT.CA Caplus document type: Patent
 RL.P Roles from patents: ANST (Analytical study); PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

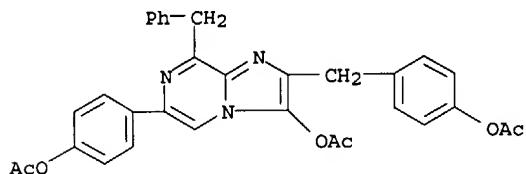
L3 ANSWER 7 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 70217-82-2 REGISTRY
 CN Imidazo[1,2-a]pyrazin-3(7H)-one, 6-phenyl-2,8-bis(phenylmethyl)- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN Bisdeoxycocleterazine
 CN Coelenterazine 400a
 CN Coelenterazine HH
 CN Dideoxycocleterazine
 FS 3D CONCORD
 MF C26 H21 N3 O
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CHEMCATS, CSCHEM, TOXCENTER, USPAT2, USPATFULL
 (*File contains numerically searchable property data)
 DT.CA Caplus document type: Journal; Patent
 RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
 RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)
 8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 8 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 65417-16-5 REGISTRY
 CN Imidazo[1,2-a]pyrazin-3-ol, 6-[4-(acetoxy)phenyl]-2-[(4-(acetoxy)phenyl)methyl]-8-(phenylmethyl)-, acetate (ester) (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C32 H27 N3 O6
 LC STN Files: BEILSTEIN*, CA, CAPLUS, USPATFULL
 (*File contains numerically searchable property data)
 DT.CA CAplus document type: Journal; Patent
 RL.P Roles from patents: ANST (Analytical study); PREP (Preparation)
 RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

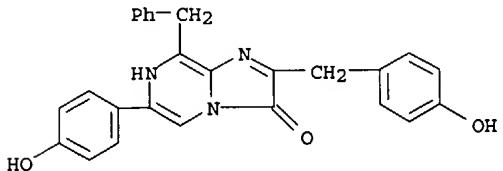
L3 ANSWER 9 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 61869-41-8 REGISTRY
 CN Luciferase (Renilla luciferin) (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN E.C. 1.13.12.5
 CN Luciferase
 CN Renilla luciferase
 CN Renilla luciferin 2-monooxygenase
 MF Unspecified
 CI MAN
 LC STN Files: ADISNEWS, AGRICOLA, BIOSIS, CA, CAPLUS, CEN, CIN, MEDLINE, PIRA, PROMT, TOX CENTER, USPAT2, USPATFULL
 DT.CA CAplus document type: Conference; Dissertation; Journal; Patent; Report
 RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)
 RLD.P Roles for non-specific derivatives from patents: ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
 RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)
 RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

205 REFERENCES IN FILE CA (1907 TO DATE)
 19 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 208 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 10 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 55779-48-1 REGISTRY
 CN Imidazo[1,2-a]pyrazin-3(7H)-one, 6-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)methyl]-8-(phenylmethyl)- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN Coelenterazin
 CN Coelenterazine
 CN Luciferin

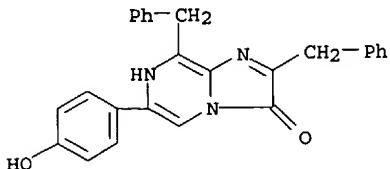
CN Luciferin (Oplophorus)
 CN NanoFuel
 CN Preluciferin
 CN Preluciferin (Watasenia)
 FS 3D CONCORD
 DR 57683-96-2
 MF C26 H21 N3 O3
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 CANCERLIT, CAPLUS, CASREACT, CEN, CHEMCATS, CIN, CSCHEM, MEDLINE, PIRA,
 PROMT, TOXCENTER, USPAT2, USPATFULL
 (*File contains numerically searchable property data)
 DT.CA CAplus document type: Conference; Journal; Patent
 RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);
 MSC (Miscellaneous); PREP (Preparation); PROC (Process); PRP
 (Properties); RACT (Reactant or reagent); USES (Uses)
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 study); BIOL (Biological study); PROC (Process); PRP (Properties); RACT
 (Reactant or reagent); USES (Uses)
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 study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU
 (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT
 (Reactant or reagent); USES (Uses); NORL (No role in record)
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 study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP
 (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

181 REFERENCES IN FILE CA (1907 TO DATE)
 22 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 181 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 11 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 50909-86-9 REGISTRY
 CN Imidazo[1,2-a]pyrazin-3(7H)-one, 6-(4-hydroxyphenyl)-2,8-bis(phenylmethyl)-
 (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 2-Deoxycoelenterazine
 CN Coelenterazine h
 CN Luciferin
 CN Luciferin (Renilla)
 FS 3D CONCORD
 DR 50815-16-2
 MF C26 H21 N3 O2
 LC STN Files: ADISNEWS, AGRICOLA, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA,
 CAPLUS, CEN, CHEMCATS, CIN, CSCHEM, MEDLINE, PIRA, PROMT, TOXCENTER,
 USPATFULL
 (*File contains numerically searchable property data)
 DT.CA CAplus document type: Conference; Journal; Patent
 RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);
 PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)
 RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological
 study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP
 (Properties); RACT (Reactant or reagent); USES (Uses)
 RLD.NP Roles for non-specific derivatives from non-patents: PREP
 (Preparation); PRP (Properties)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

40 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 40 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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FILE LAST UPDATED: 27 OCT 2004 <20041027/UP>
 MOST RECENT DERWENT UPDATE: 200469 <200469/DW>
 DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

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 HIT STRUCTURES WITHIN THE BIBLIOGRAPHIC DOCUMENT <<<

>>> SMILES and ISOSMILES strings are no longer available as
 Derwent Chemistry Resource display fields <<<

L4 ANSWER 1 OF 1 WPIX COPYRIGHT 2004 THE THOMSON CORP on STN
 AN 2003-468516 [44] WPIX
 DNN N2003-372833 DNC C2003-125061
 TI Kit useful for measuring the enzymatic activity of a luminogenic protein,
 comprises a protected luminophore and a luminogenic protein or a
 deprotecting enzyme.
 DC B02 B04 D16 S03
 IN HAWKINS, E; KLAUBERT, D; SCURRIA, M; WOOD, K
 PA (HAWK-I) HAWKINS E; (KLAU-I) KLAUBERT D; (SCUR-I) SCURRIA M; (WOOD-I) WOOD
 K; (PROM-N) PROMEGA CORP
 CYC 102
 PI WO 2003040100 A1 20030515 (200344)* EN 30 C07D211-70
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 EP 1451155 A1 20040901 (200457) EN C07D211-70
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 MK NL PT RO SE SI SK TR
 AU 2002363424 A1 20030519 (200464) C07D211-70

ADT WO 2003040100 A1 WO 2002-US34972 20021101; US 2003153090 A1 US 2001-53482 20011102; EP 1451155 A1 EP 2002-802815 20021101, WO 2002-US34972 20021101; AU 2002363424 A1 AU 2002-363424 20021101

FDT EP 1451155 A1 Based on WO 2003040100; AU 2002363424 A1 Based on WO 2003040100

PRAI US 2001-53482 20011102

IC ICM C07D211-70; G01N021-76

ICS C07D241-02; C07D413-00; C12N009-02; C12Q001-34; C12Q001-66; G01N033-53

AB WO2003040100 A UPAB: 20030710

NOVELTY - A kit comprising a protected luminophore (A) and a luminogenic protein or a deprotecting enzyme, is new.

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are included for:

(1) measurement of an enzymatic activity of a luminogenic protein involves contacting the protein, a deprotecting enzyme and (A) in a solution to form a composition (A1) and detecting the light produced from the composition;

(2) a protected luminophore which is a modified coelenterazine in which the enol group has been converted to an ester or an ether comprising an enzyme-removable group. The removal of the enzyme-removable group provides a parent coelenterazine. The time necessary for the concentration of the modified coelenterazine in a mixture comprising F12 medium and 10% fetal bovine serum at 22 deg. C to be reduced by 50% is greater than the time necessary for the concentration of the parent coelenterazine in a mixture comprising F12 medium and 10% fetal bovine serum at 22 deg. C to be reduced by 50%;

(3) generating luminescence in a living cell comprising the luciferase involves contacting the cell in solution with (A);

(4) measuring the enzymatic activity of a non-luminogenic enzyme involves contacting a liquid mixture comprising the luminogenic protein and (A) to form a composition and detecting the light produced from the composition;

(5) a compound of formula (I) - (III); and

(6) a composition comprising (I) - (III) in solution.

R7 = T or -CH2-C6H4OR14;

T = H, (hetero)alkyl or aryl;

R8 = T;

R9 = T or -C6H4OR15;

R10 = H, CH3 or -CH(CH3)2;

R11, R14 and R15 = enzyme-removable groups.

Provided that:

(1) R11, R14 and R15 are not all acetyl groups;

(2) the concentration of (I) in a mixture comprising F12 medium and 10% fetal bovine serum at 22 deg. C is reduced by less than 50% after 45 minutes;

(3) in (I), the time necessary for the concentration of the modified coelenterazine in a mixture comprising F12 medium and 10% fetal bovine serum at 22 deg. C to be reduced by 50% is greater than the time necessary for the concentration of the parent coelenterazine in a mixture comprising F12 medium and 10% fetal bovine serum at 22 deg. C to be reduced by 50% and the removal of at least one (preferably at least two, especially all) enzyme-removable groups provides the parent compound.

USE - The kit is used:

(a) for measurement of an enzymatic activity of a luminogenic protein (e.g. *Renilla* luciferase) and generating luminescence in a living cell comprising luciferase (claimed);

(b) in analytic applications e.g. to detect and quantitate luminogenic analytes which are substrates or proteins and analysis of genetic reporters e.g. multiplexed reporter where at least one reporter utilizes a luminophore;

(c) in *in vivo* applications within organism, for cell development, to measure a luminogenic analyte or non-luminogenic enzyme in a organ, tissue or cell type;

(d) in *in vitro* applications to measure substances and processed over time e.g. the expression of the luminogenic protein, the concentration of analyte and the expression of the non-luminogenic enzyme.

ADVANTAGE - The protected luminophore provides increased stability and improved signal-to-background ratio relative to the corresponding unmodified coelenterazine and provides for reduced autoluminescence under normal use conditions and is sensitive to substances other than luminogenic proteins. Therefore the composition is multi-functional and so provides a way to analyze non-luminogenic substances or processes through luminescent methods.

Dwg.0/3

FS CPI EPI

FA AB; GI; DCN

MC CPI: B04-F01; B04-L01; B04-L03C; B04-N04; B06-D08; B06-D18; B11-C07B4;
B12-K04E; D05-A01A4; D05-A01B; D05-H09
EPI: S03-E14H4
M1 *01* DCN: RA00GT-K; RA00GT-Z
M1 *02* DCN: RA0F7A-K; RA0F7A-A; RA0F7A-M
M1 *03* DCN: RA00H3-K; RA00H3-A; RA00H3-M
M1 *04* DCN: RA00GC-K; RA00GC-A; RA00GC-M
M2 *05* DCN: RAAOUX-K; RAAOUX-D; RAAOUX-M
M2 *06* DCN: 0095-66101-K; 0095-66101-D; 0095-66101-M

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FILE 'HOME' ENTERED AT 08:32:33 ON 01 NOV 2004

=>

~~=> b req~~

ENTERED AT 09:27:54 ON 01 NOV 2004
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Property values tagged with IC are from the ZIC/VINITI data file
 provided by InfoChem.

STRUCTURE FILE UPDATES: 29 OCT 2004 HIGHEST RN 772333-32-1
 DICTIONARY FILE UPDATES: 29 OCT 2004 HIGHEST RN 772333-32-1

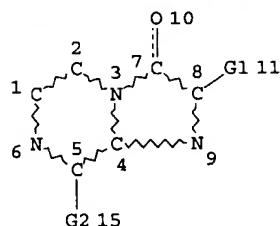
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
 information enter HELP PROP at an arrow prompt in the file or refer
 to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

[REDACTED]



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Cy @16

VAR G1=H/AK/16/12
 VAR G2=H/AK/16

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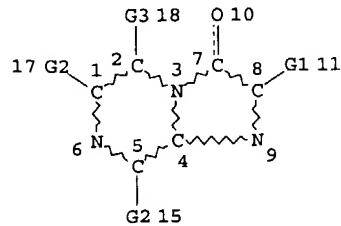
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 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS E6 C AT 13

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L7 52 SEA FILE=REGISTRY SSS FUL L5
 L8 STR



G3 18 O 10
 Ak-Cb==O
 @12 13 14

Formula XII

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VAR G2=H/AK/16

VAR G3=H/AK

NODE ATTRIBUTES:

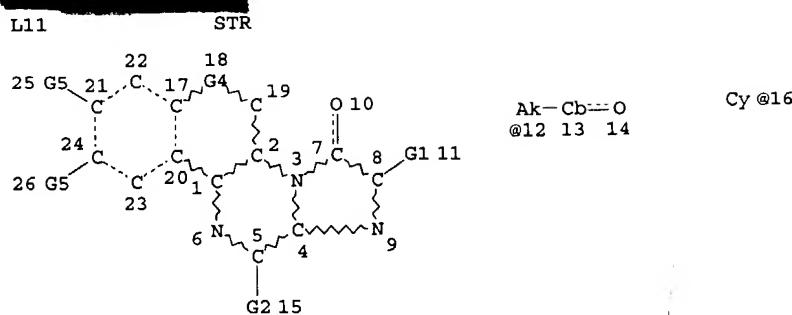
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 DEFAULT MLEVEL IS ATOM
 GGCAT IS MCY UNS AT 13
 GGCAT IS UNS AT 16
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS E6 C AT 13

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

100.0% PROCESSED 52 ITERATIONS
SEARCH TIME: 00.00.01

Formula

XIII 6c

XIV

VAR G1=H/AK/16/12

VAR G2=H/AK/16

REP G4=(0-2) C

VAR G5=H/O/AK/16

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS MCY UNS AT 13

GGCAT IS UNS AT 16

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS E6 C AT 13

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE

100.0% PROCESSED 2895 ITERATIONS
SEARCH TIME: 00.00.01

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FILE 'HCAPLUS' ENTERED AT 08:30:55 ON 01 NOV 2004

L1 1 US20030153090/PN

FILE 'REGISTRY' ENTERED AT 08:31:20 ON 01 NOV 2004

FILE 'HCAPLUS' ENTERED AT 08:31:23 ON 01 NOV 2004

L2 TRA L1 1- RN : 11 TERMS

FILE 'REGISTRY' ENTERED AT 08:31:24 ON 01 NOV 2004

L3 11 SEA L2

FILE 'WPIX' ENTERED AT 08:31:37 ON 01 NOV 2004

L4 1 US20030153090/PN

FILE 'REGISTRY' ENTERED AT 08:55:54 ON 01 NOV 2004

L5 STR

L6 5 L5

L7 52 L5 FULL

SAVE TEMP GIT482F0/A L7

L8 STR L5

L9 2 L8 SAM SUB=L7
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 L11 STR L5
 L12 0 L11 SAM SUB=L7
 L13 0 L11
 [REDACTED]

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 L16 0 L10

[REDACTED] ENTERED AT 09:22:40 ON 01 NOV 2004
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 E WOOD KEITH/AU
 L18 113 E3-9
 E HAWKINS E/AU
 L19 78 E3-15
 E HAWKINS ERICA/AU
 E HAWKINS ERIKA/AU
 L20 8 E3-4
 E SCURRIA M/AU
 L21 4 E4-7
 E KLAUBERT D/AU
 L22 68 E4-8
 L23 249 PROMEGA/CS, PA
 L24 3 L15 AND L17-22
 L25 3 L15 AND L23

L27 23 L15 NOV L26

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 [REDACTED] ENTERED AT 09:28:14 ON 01 NOV 2004
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FILE COVERS 1907 - 1 Nov 2004 VOL 141 ISS 19
 FILE LAST UPDATED: 31 Oct 2004 (20041031/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

[REDACTED]
 L26 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 2004:270174 HCAPLUS
 DN 140:299425
 ED Entered STN: 02 Apr 2004
 TI Luminescent cytochrome P 450 assay using luciferase, luciferin derivatives and pyrophosphatase, and drug screening applications
 [REDACTED] Cali, James J.; Klaubert, Dieter; Daily, William; Ho, Samuel Kin Sang; Frackman, Susan; Hawkins, Erika; Wood, Keith V.
 [REDACTED] Promega Corporation, USA
 SO PCT Int. Appl., 130 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 IC ICM G01N
 CC 7-1 (Enzymes)

Section cross-reference(s): 1, 63

| FAN.CNT 1 | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------|---|------|----------|-----------------|----------|
| PI | WO 2004027378 | A2 | 20040401 | WO 2003-US29078 | 20030916 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU | | | | |
| | RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| | US 2004171099 | A1 | 20040902 | US 2003-665314 | 20030919 |
| PRAI | US 2002-412254P | P | 20020920 | | |
| | US 2003-483309P | P | 20030627 | | |

CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|---------------|-------|------------------------------------|
| WO 2004027378 | ICM | G01N |

OS MARPAT 140:299425

AB The present invention provides methods, compns., substrates, and kits useful for analyzing the metabolic activity in cells, tissue, and animals and for screening test compds. for their effect on cytochrome P 450 activity. In particular, a one-step and two-step methods using luminogenic mols., e.g. luciferin or coelenterazines, that are cytochrome P 450 substrates and that are also bioluminescent enzyme, e.g., luciferase, pro-substrates are provided. Upon addition of the luciferin derivative or other luminogenic mol. into a P 450 reaction, the P 450 enzyme metabolizes the mol. into a bioluminescent enzyme substrate, e.g., luciferin and/or luciferin derivative metabolite, in a P 450 reaction. The resulting metabolite(s) serves as a substrate of the bioluminescent enzyme, e.g., luciferase, in a second light-generating reaction. Luminescent cytochrome P 450 assays with low background signals and high sensitivity are disclosed and isoform selectivity is demonstrated. The present invention also provides an improved method for performing luciferase reactions which employs added pyrophosphatase to remove inorg. pyrophosphate, a luciferase inhibitor which may be present in the reaction mixture as a contaminant or may be generated during the reaction. The present method further provides a method for stabilizing and prolonging the luminescent signal in a luciferase-based assay using luciferase stabilizing agents such as reversible luciferase inhibitors.

ST cytochrome P 450 detn luciferase luciferin coelenterazine bioluminescence; drug screening cytochrome P 450 luminescent assay

IT Animal

Animal tissue

Bile

Cell

Feces

Liver

Microsome

(P 450 determination in; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT Transgene

RL: BPN (Biosynthetic preparation); BUU (Biological use, unclassified); BIOL (Biological study); PREP (Preparation); USES (Uses)
(animal, P 450 determination in; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT Enzymes, uses

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(bioluminescent; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT High throughput screening

(drug; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT Drug screening

(high throughput; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT Teleostei

(in high throughput screening assay; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT Blood analysis
 Chemiluminescence spectroscopy
 Chemiluminescent substances
 Cytolysis
 High throughput screening
 Luminescence, bioluminescence
 Luminescence spectroscopy
 Luminescent substances
 Surfactants
 Test kits
 Urine analysis
 (luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT Surfactants
 (nonionic; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 7048-04-6, Cysteine hydrochloride monohydrate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (conversion of 2-cyanobenzothiazole derivs. to D-luciferin derivs.; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 9035-51-2, Cytochrome P 450, biological studies
 RL: ANT (Analyte); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
 (luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 56-65-5, 5'-ATP, uses 2591-17-5D, Luciferin, derivs. 7439-95-4, Magnesium, uses 55779-48-1, Coelenterazine 55779-48-1D, Coelenterazine, derivs. 676460-49-4D, Imidazo[1,2-a]pyrazin-3-ol, derivs.
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
 (luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 9014-00-0P, Luciferase 61869-41-8P, Renilla luciferase 61970-00-1P, Firefly luciferase
 RL: ARG (Analytical reagent use); BPN (Biosynthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 676460-30-3P 676460-31-4P 676460-32-5P 676460-33-6P 676460-34-7P
 676460-35-8P 676460-37-0P 676460-39-2P 676460-41-6P 676460-43-8P
 676460-47-2P, Coelenterazine HH methyl ether
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
 (luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 9024-82-2, Pyrophosphatase
 RL: ARU (Analytical role, unclassified); ANST (Analytical study)
 (luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 100-39-0, Benzyl bromide 107-04-0, 1-Bromo-2-chloroethane 402-49-3, 4-(Trifluoromethyl)benzyl bromide 615-20-3, 2-Chlorobenzothiazole 870-63-3, Prenyl bromide 939-69-5, 2-Cyano-6-hydroxybenzothiazole 2591-17-5, D-Luciferin 4916-55-6, 3-(Bromomethyl)pyridine hydrobromide 6138-90-5, Geranyl bromide 31106-82-8, 2-(Bromomethyl)pyridine hydrobromide 73870-24-3, 4-(Bromomethyl)pyridine hydrobromide
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of 2-cyanobenzothiazole derivs.; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 103-63-9P, 2-(Bromoethyl)benzene 2602-85-9P, 2-Cyanobenzothiazole 676460-20-1P 676460-21-2P 676460-22-3P 676460-23-4P 676460-24-5P
 676460-25-6P 676460-26-7P 676460-27-8P 676460-28-9P 676460-29-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of 2-cyanobenzothiazole derivs.; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 70217-82-2P, Coelenterazine HH
 RL: ARG (Analytical reagent use); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (preparation of coelenterazine derivs.; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

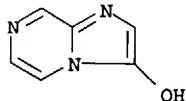
IT 79-37-8, Oxalyl chloride 108-24-7, Acetic anhydride 156-06-9, Phenylpyruvic acid 17476-04-9, Lithium tri-tert-butoxyaluminohydride 70217-86-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of coelenterazine derivs.; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 56485-04-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of coelenterazine derivs.; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 92-36-4, 2-(4-Aminophenyl)-6-methylbenzothiazole 2536-91-6, 2-Amino-6-methylbenzothiazole
 RL: ARU (Analytical role, unclassified); ANST (Analytical study)
 (stabilization of luminescent signal using luciferase inhibitor; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 676460-49-4D, Imidazo[1,2-a]pyrazin-3-ol, derivs.
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
 (luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

RN 676460-49-4 HCAPLUS
 CN Imidazo[1,2-a]pyrazin-3-ol (9CI) (CA INDEX NAME)



L26 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 2003:376823 HCAPLUS
 DN 138:365147
 ED Entered STN: 16 May 2003
 TI Compositions, methods and kits pertaining to luminescent compounds
 IN Wood, Keith; Hawkins, Erika; Scurria, Mike;
 Klaubert, Dieter
 PA Promega Corporation, USA
 SO PCT Int. Appl., 60 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 IC ICM C07D211-70
 ICS C07D241-02; C07D413-00; C12N009-02; C12Q001-34; C12Q001-66;
 G01N033-53
 CC 9-14 (Biochemical Methods)
 Section cross-reference(s): 80

FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| PI WO 2003040100 | A1 | 20030515 | WO 2002-US34972 | 20021101 |
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| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 2003153090 | A1 | 20030814 | US 2001-53482 | 20011102 |
| EP 1451155 | A1 | 20040901 | EP 2002-802815 | 20021101 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK | | | | |
| PRAI US 2001-53482 | A | 20011102 | | |
| WO 2002-US34972 | W | 20021101 | | |

CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|------------|-------|------------------------------------|
|------------|-------|------------------------------------|

WO 2003040100 ICM C07D211-70
 ICS C07D241-02; C07D413-00; C12N009-02; C12Q001-34;
 C12Q001-66; G01N033-53

OS MARPAT 138:365147
 AB A method of measuring the enzymic activity of a luciferase includes contacting a luminogenic protein, such as a luciferase, with a protected luminophore to form a composition; and detecting light produced from the composition. The protected luminophore provides increased stability and improved signal-to-background ratios relative to the corresponding unmodified coelenterazine.

ST compn kit pertaining luminescent compd protein

IT Cell

Luminescent substances

(compns., methods and kits pertaining to luminescent compds.)

IT Proteins

RL: ARU (Analytical role, unclassified); ANST (Analytical study)
 (luminogenic; compns., methods and kits pertaining to luminescent compds.)

IT 61869-41-8, Renilla luciferase

RL: ARU (Analytical role, unclassified); ANST (Analytical study)
 (compns., methods and kits pertaining to luminescent compds.)

IT 50909-86-9P 55779-48-1P 65417-16-5P 70217-82-2P

524066-91-9P 524066-92-0P 524066-93-1P

524066-94-2P 524066-95-3P 524066-96-4P

RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)

(compns., methods and kits pertaining to luminescent compds.)

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Bryan; US 6416960 B1 2002 HCPLUS

(2) Garini; US 6165734 A 2000 HCPLUS

(3) Hideshi, N; Journal American Chem Society 2001, V123, P1523

(4) Inouye, S; Biochemical and Biophysical Research Communications 1997, V233, P349 HCPLUS

(5) Jones, K; Trends in Biotechnology 1999, V17, P477 HCPLUS

(6) Roelant; US 6171809 B1 2001 HCPLUS

(7) Shimomura, O; Biochemistry Journal 1989, V261, P913 HCPLUS

(8) Shimomura, O; Biochemistry Journal 1995, V306, P537 HCPLUS

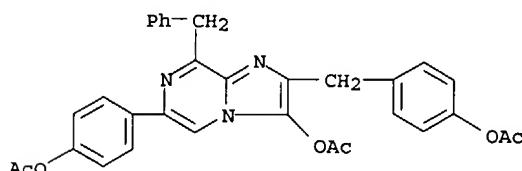
IT 65417-16-5P

RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)

(compns., methods and kits pertaining to luminescent compds.)

RN 65417-16-5 HCPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 6-[4-(acetoxy)phenyl]-2-[[4-(acetoxy)phenyl]methyl]-8-(phenylmethyl)-, acetate (ester) (9CI) (CA INDEX NAME)



L26 ANSWER 3 OF 3 HCPLUS COPYRIGHT 2004 ACS on STN

AN 2003:108790 HCPLUS

DN 139:129758

ED Entered STN: 12 Feb 2003

TI Coelenterazine derivatives for improved solution solubility

AU Hawkins, Erika M.; O'Grady, Michael; Klaubert, Dieter;
 Scurria, Michael; Good, Troy; Stratford, Cathy; Flemming, Rod;
 Simpson, Dan; Wood, Keith V.

CS Promega Corporation, Madison, WI, 53715, USA

SO Bioluminescence & Chemiluminescence: Progress & Current Applications, [Proceedings of the Symposium on Bioluminescence and Chemiluminescence], 12th, Cambridge, United Kingdom, Apr. 5-9, 2002 (2002), 149-152.
 Editor(s): Stanley, Philip E.; Kricka, Larry J. Publisher: World Scientific Publishing Co. Pte. Ltd., Singapore, Singapore.
 CODEN: 69DPGZ; ISBN: 981-238-156-2

DT Conference

LA English

CC 7-3 (Enzymes)
 Section cross-reference(s): 9

AB Intracellular luminescent techniques requiring coelenterazine, such as bioluminescence resonance energy transfer (BRET), calcium detection, and intracellular reporter measurements, must accommodate the poor stability of this substrate in physiol. buffered solns. Coelenterazine degradation leads both to loss of luminescence over time, and increased background luminescence caused by enzyme-independent oxidation (autoluminescence). Both conditions limit luminescence sensitivity by reducing the signal-to-noise ratio. Coelenterazine can be stabilized by derivatizing the enol oxygen with an acyl oxymethyl ether. This prevents spontaneous oxidation in solution while making the substrate available intracellularly upon cleavage of the blocking group by endogenous esterases. We will describe the stability of pivaloyl oxymethyl coelenterazine-h (POM coelenterazine-h), and the effect of POM coelenterazine-h on intracellular luminescence, autoluminescence, and luminescent reaction kinetics. Also, we will present the characteristics of two other coelenterazine derivs.

ST coelenterazine deriv improved soln soly reporter

IT Luminescence
 (coelenterazine derivs. for improved solution solubility)

IT Animal cell line
 (mammalian; coelenterazine derivs. for improved solution solubility)

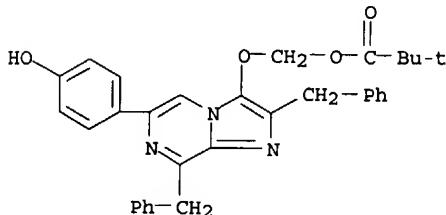
IT 50909-86-9, Coelenterazine-h 61869-41-8, Renilla luciferase
 524066-95-3D, diacetyl derivative 566945-96-8
 RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

IT 524066-95-3D, diacetyl derivative
 RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

IT (coelenterazine derivs. for improved solution solubility)

RN 524066-95-3 HCPLUS

CN Propanoic acid, 2,2-dimethyl-, [[6-(4-hydroxyphenyl)-2,8-bis(phenylmethyl)imidazo[1,2-a]pyrazin-3-yl]oxy]methyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 1 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
 AN 2001:851130 HCPLUS
 DN 135:371764
 ED Entered STN: 23 Nov 2001
 TI Preparation of aminopyrazines and imidazolopyrazinones as antioxidants
 IN Marchand-Brynaert, Jacqueline; Cavalier, Jean-Francois; Rees, Jean-Francois; De Tollenaere, Catherine; Burton, Maggi
 PA Universite Catholique de Louvain, Belg.
 SO PCT Int. Appl., 57 pp.
 CODEN: PIXXD2

DT Patent
 LA English
 IC ICM C07D241-20
 ICS A61K031-495; A23L003-3544; C08K005-3462
 CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 1, 17, 38, 62

FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|--------------|
| PI WO 2001087853 | A1 | 20011122 | WO 2001-EP5588 | 20010516 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, | | | | |

LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
 SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
 YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
 EP 1292580 A1 20030319 EP 2001-943383 20010516 <--
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
 US 2004034225 A1 20040219 US 2003-276398 20030728 <--
 PRAI EP 2000-870107 A 20000517 <--
 EP 2000-870293 A 20001212 <--
 WO 2001-EP5588 W 20010516 <--

CLASS

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

 WO 2001087853 ICM C07D241-20
 ICS A61K031-495; A23L003-3544; C08K005-3462
 US 2004034225 ECLA A23L003/3544; C07D241/20; C07D487/04 <--
 OS CASREACT 135:371764; MARPAT 135:371764

AB Antioxidants, 5 2-amino-(p-hydroxyphenyl)pyrazines and 3 (p-hydroxyphenyl)-3,7-dihydroimidazo[1,2-a]pyrazin-3-ones were prepared and claimed useful in diagnostic procedures, as food additives, polymer additives and as UV screens in cosmetics. E.g., 2-amino-3,5-dibromopyrazine was treated with p-methoxyphenylboronic acid in the presence of bis(benzonitrile)palladium dichloride and 1,4-bis(diphenylphosphino)butane in a solvent mix of EtOH, aqueous sodium carbonate and toluene to give 66% 2-amino-3,5-bis(p-methoxyphenyl)pyrazine, which was demethylated with Et3N in DMF to give 88% 2-amino-3,5-bis(p-hydroxyphenyl)pyrazine (I). In tests on inhibition of lipid peroxidn. 2-aminopyrazines possessing 2 aryl substituents, one of them being a p-hydroxyphenyl in o- or p- position with respect to the amino group, are endowed with antioxidative properties. However, the p-hydroxyphenyl conferred more activity when located at position 5 than at position 3. The presence of p-hydroxyphenyl groups at both positions 3 and 5 as in I produced a very active compound. Analogs lacking the free phenol groups showed reduced activities. Corresponding imidazolopyrazinones combined the properties of both the imidazolopyrazinones (delay of the onset of peroxidn.) and the aminopyrazines (lower rate of oxidation after onset).

ST antioxidant aminopyrazine imidazolopyrazinone prep; food additive antioxidant aminopyrazine imidazolopyrazinone prep; polymer additive antioxidant aminopyrazine imidazolopyrazinone prep; lipid peroxidn inhibitor antioxidant aminopyrazine imidazolopyrazinone prep; UV screen cosmetic antioxidant aminopyrazine imidazolopyrazinone prep; pyrazine amino hydroxyphenyl prep

IT Azines

RL: FFD (Food or feed use); MOA (Modifier or additive use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 ((p-hydroxyphenyl)pyrazines; preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT Polymers, uses

RL: POF (Polymer in formulation); USES (Uses)
 (additives; preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT Azines

RL: FFD (Food or feed use); MOA (Modifier or additive use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (aminopyrazines; preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT Lipids, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)
 (peroxidn.; preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT UV B radiation

(preparation of aminopyrazines and imidazolopyrazinones as antioxidant protectants against)

IT Sunscreens

(preparation of aminopyrazines and imidazolopyrazinones as antioxidant protectants against UVB radiation)

IT Antioxidants

Food additives

Food preservatives

(preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT 350230-59-0P, 2,6-Diamino-3,5-bis(p-hydroxyphenyl)pyrazine 350230-62-5P, 2-Amino-3,5-bis(p-hydroxyphenyl)pyrazine 374588-71-3P, 2-Amino-5-(p-hydroxyphenyl)-3-methylpyrazine 374588-73-5P, 2-Amino-3-(p-hydroxyphenyl)-5-phenylpyrazine
 RL: FFD (Food or feed use); MOA (Modifier or additive use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT 350230-61-4P 374588-74-6P 374588-75-7P 374588-76-8P 374588-77-9P 374588-78-0P
 RL: FFD (Food or feed use); MOA (Modifier or additive use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT 19943-97-6P 27955-58-4P
 RL: FFD (Food or feed use); MOA (Modifier or additive use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT 98-80-6, Phenylboronic acid 100-39-0, Benzyl bromide 5720-07-0, p-Methoxyphenylboronic acid 24241-18-7, 2-Amino-3,5-dibromopyrazine 58885-20-4, 2,6-Diamino-3,5-dibromopyrazine 59489-71-3, 2-Amino-5-bromopyrazine 67602-05-5, 2-Amino-3-bromo-5-phenylpyrazine 122775-35-3, 3,4-Dimethoxyphenylboronic acid 350819-24-8, 2-Amino-3-bromo-5-(4-methoxyphenyl)pyrazine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT 350230-58-9P, 2,6-Diamino-3,5-bis(p-methoxyphenyl)pyrazine 350819-13-5P 350819-14-6P 374588-70-2P, 2-Amino-5-(p-methoxyphenyl)-3-methylpyrazine 374588-72-4P, 2-Amino-3-(p-methoxyphenyl)-5-phenylpyrazine 374588-81-5P 374588-83-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT 119738-50-0P, 2-Amino-5-(4-methoxyphenyl)pyrazine 174680-63-8P, 2-Amino-3,5-bis(p-methoxyphenyl)pyrazine
 RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT 57683-97-3P 123488-68-6P 123488-69-7P 144763-52-0P 152719-89-6P 152719-90-9P 152916-61-5P 350819-19-1P 374588-79-1P 374588-80-4P 374588-82-6P 374588-84-8P 374588-85-9P 374588-86-0P 374588-87-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT 13535-13-2P, 2-Amino-5-phenylpyrazine 41270-70-6P, 2-Amino-3,5-diphenylpyrazine 73444-23-2P, 2-Methylamino-5-phenylpyrazine 204770-67-2P, 2-Amino-5-(4-hydroxyphenyl)pyrazine
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

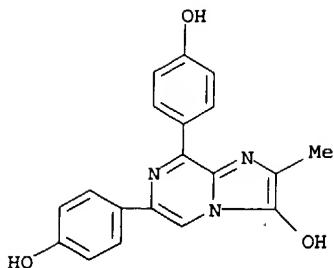
RE

- (1) Anon; PATENT ABSTRACTS OF JAPAN 1996, V1996(07)
- (2) Anon; PATENT ABSTRACTS OF JAPAN 1997, V1997(03)
- (3) Anon; PATENT ABSTRACTS OF JAPAN 1998, V1998(08)
- (4) Dubuisson, M; WO 9843641 A 1998 HCPLUS
- (5) Nippon Oil & JP 08059686 A 1996 HCPLUS
- (6) Nippon Oil & JP 08294397 A 1996 HCPLUS
- (7) Nippon Shokuhin Kako Co Ltd; JP 10077286 A 1998 HCPLUS
- (8) Sato; SYNTHESIS 1994, V9, P931
- (9) Univ Louvain; WO 9628160 A 1996 HCPLUS
- (10) Watanabe; SYNTHESIS 1980, V1, P39 MEDLINE

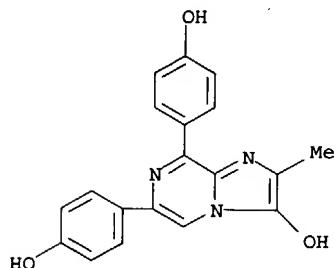
IT 374588-75-7P 374588-76-8P 374588-77-9P
 374588-78-0P
 RL: FFD (Food or feed use); MOA (Modifier or additive use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

RN 374588-75-7 HCPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 6,8-bis(4-hydroxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)

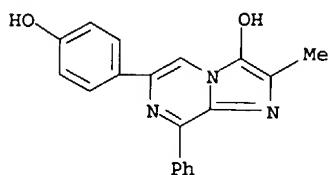


RN 374588-76-8 HCPLUS
 CN Imidazo[1,2-a]pyrazin-3-ol, 6,8-bis(4-hydroxyphenyl)-2-methyl-,
 monohydrochloride (9CI) (CA INDEX NAME)

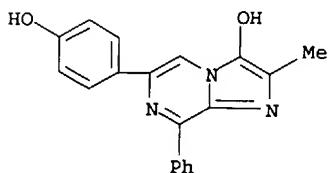


● HCl

RN 374588-77-9 HCPLUS
 CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2-methyl-8-phenyl- (9CI)
 (CA INDEX NAME)



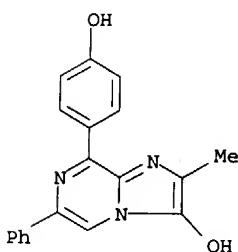
RN 374588-78-0 HCPLUS
 CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2-methyl-8-phenyl-,
 monohydrochloride (9CI) (CA INDEX NAME)



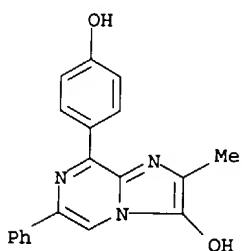
● HCl

IT 374588-79-1P 374588-80-4P 374588-85-9P
 374588-86-0P 374588-87-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

RN 374588-79-1 HCAPLUS
 CN Imidazo[1,2-a]pyrazin-3-ol, 8-(4-hydroxyphenyl)-2-methyl-6-phenyl- (9CI)
 (CA INDEX NAME)

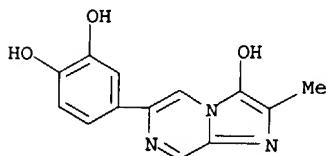


RN 374588-80-4 HCAPLUS
 CN Imidazo[1,2-a]pyrazin-3-ol, 8-(4-hydroxyphenyl)-2-methyl-6-phenyl-,
 monohydrochloride (9CI) (CA INDEX NAME)

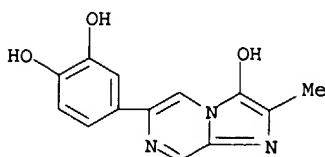


● HCl

RN 374588-85-9 HCAPLUS
 CN 1,2-Benzenediol, 4-(3-hydroxy-2-methylimidazo[1,2-a]pyrazin-6-yl)- (9CI)
 (CA INDEX NAME)

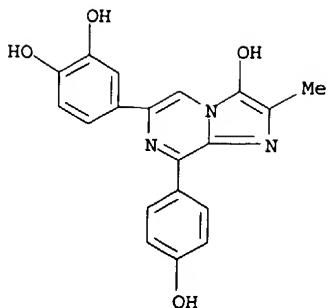


RN 374588-86-0 HCAPLUS
 CN 1,2-Benzenediol, 4-(3-hydroxy-2-methylimidazo[1,2-a]pyrazin-6-yl)-,
 monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 374588-87-1 HCAPLUS
 CN 1,2-Benzenediol, 4-[3-hydroxy-8-(4-hydroxyphenyl)-2-methylimidazo[1,2-a]pyrazin-6-yl]- (9CI) (CA INDEX NAME)



L28 ANSWER 2 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
 AN 1997:48722 HCPLUS
 DN 126:72331
 ED Entered STN: 23 Jan 1997
 TI Chemiluminescent substrate for enzyme immunoassay
 IN Sakaki, Hidejiro; Mitani, Motohiro; Koinuma, Yasuyoshi; Totani, Yoshiaki
 PA Nippon Oils & Fats Co Ltd, Japan
 SO Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC ICM C12Q001-34
 ICS G01N021-78; G01N033-543
 CC 9-10 (Biochemical Methods)
 FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------------|------|----------|-----------------|--------------|
| PI JP 08294397 | A2 | 19961112 | JP 1995-125617 | 19950427 <-- |
| PRAI JP 1995-125617 | | 19950427 | | |

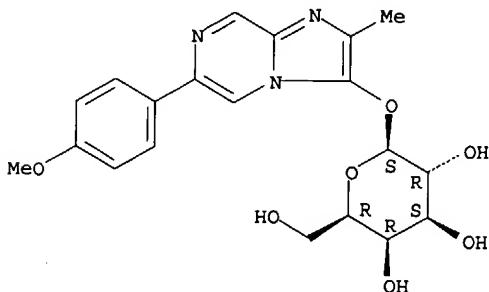
CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|-------------|-------|------------------------------------|
| JP 08294397 | ICM | C12Q001-34 |
| | | ICS G01N021-78; G01N033-543 |

OS MARPAT 126:72331
 AB Chemiluminescent substrate for sugar-hydrolyzing enzyme is prepared for EIA. 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazole[1,2-alpha]pyrazine was prepared from 6-(4-methoxyphenyl)-2-methyl-3-(tetra-O-acetyl-.beta.-D-galactopyranosyloxy)imidazole[1,2-a]pyrazine, and used for chemiluminescent EIA.
 ST chemiluminescence EIA substrate carbohydrate hydrolyzing enzyme
 IT Immunoglobulins
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
 (G, galactosidase; chemiluminescent substrate for EIA using carbohydrate-hydrolyzing enzyme)
 IT Immunoassay
 Immunoassay
 (chemiluminescence enzyme; chemiluminescent substrate for EIA using carbohydrate-hydrolyzing enzyme)
 IT 9001-02-9, Carbohydrate-hydrolyzing enzymes 9031-11-2,
 .beta.-Galactosidase
 RL: ARU (Analytical role, unclassified); ANST (Analytical study)
 (chemiluminescent substrate for EIA using carbohydrate-hydrolyzing enzyme)
 IT 159503-66-9P
 RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)
 (chemiluminescent substrate for EIA using carbohydrate-hydrolyzing enzyme)
 IT 3068-32-4, 2,3,4,6-Tetra-O-acetyl-.alpha.-D-galactopyranosyl bromide
 185311-71-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (chemiluminescent substrate for EIA using carbohydrate-hydrolyzing enzyme)
 IT 177205-13-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (chemiluminescent substrate for EIA using carbohydrate-hydrolyzing

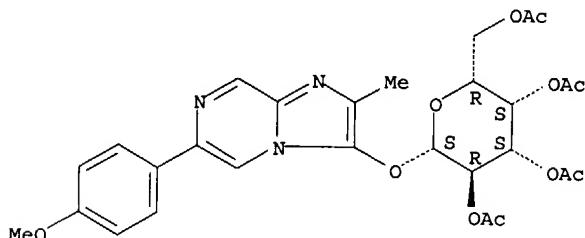
enzyme)
 IT 159503-66-9P
 RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST
 (Analytical study); PREP (Preparation)
 (chemiluminescent substrate for EIA using carbohydrate-hydrolyzing
 enzyme)
 RN 159503-66-9 HCPLUS
 CN .beta.-D-Galactopyranoside, 6-(4-methoxyphenyl)-2-methylimidazo[1,2-
 a]pyrazin-3-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 177205-13-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (chemiluminescent substrate for EIA using carbohydrate-hydrolyzing
 enzyme)
 RN 177205-13-9 HCPLUS
 CN .beta.-D-Galactopyranoside, 6-(4-methoxyphenyl)-2-methylimidazo[1,2-
 a]pyrazin-3-yl, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 3 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
 AN 1996:335963 HCPLUS
 DN 125:11354
 ED Entered STN: 08 Jun 1996
 TI Preparation of luciferin derivatives of Umihotaru (Cypridina hilgendorfii)
 IN Mitani, Motohiro; Sakaki, Hidejiro; Koinuma, Yasuyoshi; Totani, Yoshiaki
 PA Nippon Oils & Fats Co Ltd, Japan
 SO Jpn. Kokai Tokkyo Koho, 8 pp.
 CODEN: JKXXAF

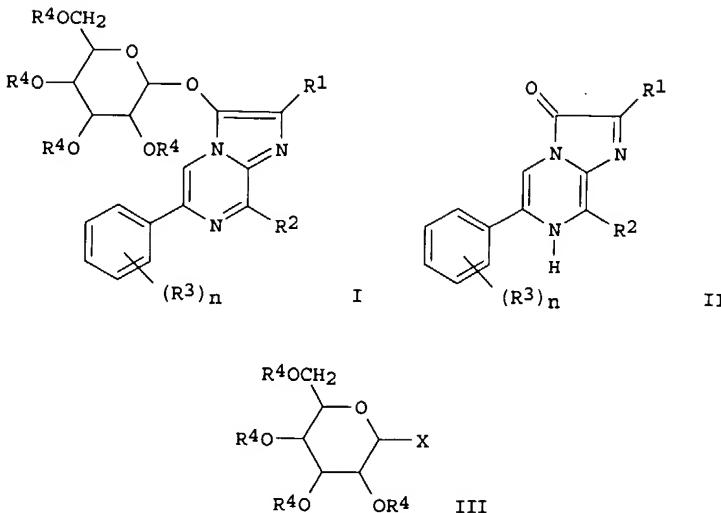
DT Patent
 LA Japanese
 IC ICM C07H017-02
 ICS C07D487-04; C12Q001-34; G01N021-78
 CC 33-3 (Carbohydrates)
 Section cross-reference(s): 9
 FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------------|-------|----------|-----------------|--------------|
| ----- | ----- | ----- | ----- | ----- |
| PI JP 08059686 | A2 | 19960305 | JP 1994-198770 | 19940823 <-- |
| PRAI JP 1994-198770 | | 19940823 | | <-- |

 CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|-------------|-------|------------------------------------|
| ----- | ----- | ----- |
| JP 08059686 | ICM | C07H017-02 |

OS ICS C07D487-04; C12Q001-34; G01N021-78
 OS CASREACT 125:11354; MARPAT 125:11354
 GI



AB The title compds. (I; R1, R2 = H, C1-20 alkyl, C6-20 aryl, C7-19 arylalkyl; R3 = C1-5 alkyl or alkoxy; n = 0-5), which are useful as substrates for luminescent determination of sugar hydrolases such as .alpha.-D-galactosidase, are prepared by reacting imidazopyrazinone derivs. (III; R1 - R3, n = same as above) with sugar derivs. (III; X = halo; R4 = C1-7 acyl) in the presence of silver triflate and Na2HPO4. followed by solvolysis in the presence of an alkali. Thus, 0.1 g 6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazin-3-one and 1.1 g Na2HPO4 were treated with 5 mL MeCN, 9 mL benzene, and 2.6 g mol. sieve 4A and stirred at room temperature for 1 h, treated with 0.18 g 2,3,4,6-tetra-O-acetyl-.alpha.-D-galactopyranosyl bromide and 0.37 g silver triflate, and stirred at room temperature for 2 h to give 39% 6-(4-methoxyphenyl)-2-methyl-3-(2,3,4,6-tetra-O-acetyl-.alpha.-D-galactopyranosyloxy)imidazo[1,2-a]pyrazine, which (0.5 g) was treated with 3.5 mL MeOH and 1.8 mL concentrated aqueous NH3 and stirred at 40.degree. for 6 h 30 min to give 78% 6-(4-methoxyphenyl)-2-methyl-3-(.alpha.-D-galactopyranosyloxy)imidazo[1,2-a]pyrazine (IV). IV showed luminescence in the presence of .beta.-D-galactosidase with correlation factor r = 0.992.

ST luciferin deriv Cypridina hilgendorfii prepn; luminescent detn sugar hydrolase; galactosidase luminescent detn substrate luciferin deriv; glucosidase luminescent detn; imidazopyrazinone glycosidation; silver triflate glycosidation catalyst; disodium hydrogen phosphate glycosidation catalyst

IT Luminescence
 (preparation of luciferin derivs. of Cypridina hilgendorfii as substrates for luminescent determination of sugar hydrolases)

IT Glycosidation catalysts
 (silver triflate and disodium hydrogen phosphate for preparation of luciferin derivs. of Cypridina hilgendorfii by glycosidation of imidazopyrazinones as substrates for luminescent determination of sugar hydrolases)

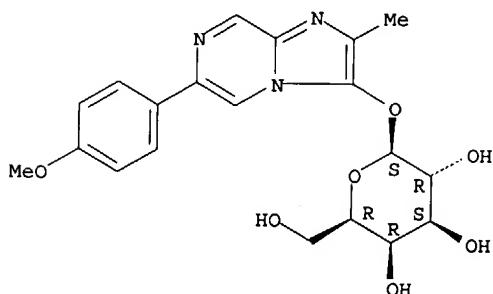
IT 9031-11-2
 RL: ANT (Analyte); ANST (Analytical study)
 (preparation of luciferin derivs. of Cypridina hilgendorfii as substrates for luminescent determination of sugar hydrolases)

IT 159503-66-9P 177205-12-8P
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
 (preparation of luciferin derivs. of Cypridina hilgendorfii as substrates for luminescent determination of sugar hydrolases)

IT 2923-28-6, Silver triflate 3068-32-4, 2,3,4,6-Tetra-O-acetyl-.alpha.-D-galactopyranosyl bromide 7558-79-4, Disodium hydrogen phosphate
 RL: CAT (Catalyst use); USES (Uses)
 (preparation of luciferin derivs. of Cypridina hilgendorfii as substrates

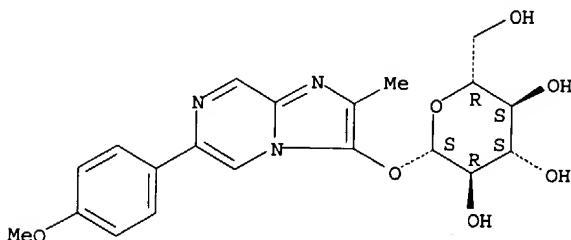
IT for luminescent determination of sugar hydrolases
 572-09-8, 2,3,4,6-Tetra-O-acetyl-.alpha.-D-glucopyranosyl bromide
 118877-07-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of luciferin derivs. of Cypridina hilgendorfii as substrates
 for luminescent determination of sugar hydrolases)
 IT 177205-13-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of luciferin derivs. of Cypridina hilgendorfii as substrates
 for luminescent determination of sugar hydrolases)
 IT 159503-66-9P 177205-12-8P
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST
 (Analytical study); PREP (Preparation); USES (Uses)
 (preparation of luciferin derivs. of Cypridina hilgendorfii as substrates
 for luminescent determination of sugar hydrolases)
 RN 159503-66-9 HCPLUS
 CN .beta.-D-Galactopyranoside, 6-(4-methoxyphenyl)-2-methylimidazo[1,2-
 a]pyrazin-3-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



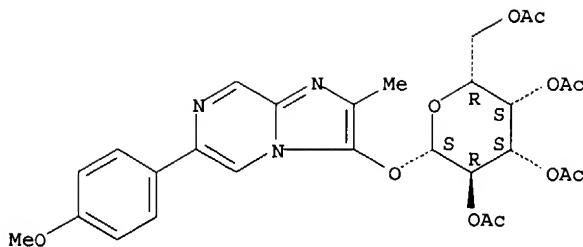
RN 177205-12-8 HCPLUS
 CN .beta.-D-Glucopyranoside, 6-(4-methoxyphenyl)-2-methylimidazo[1,2-
 a]pyrazin-3-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 177205-13-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of luciferin derivs. of Cypridina hilgendorfii as substrates
 for luminescent determination of sugar hydrolases)
 RN 177205-13-9 HCPLUS
 CN .beta.-D-Galactopyranoside, 6-(4-methoxyphenyl)-2-methylimidazo[1,2-
 a]pyrazin-3-yl, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

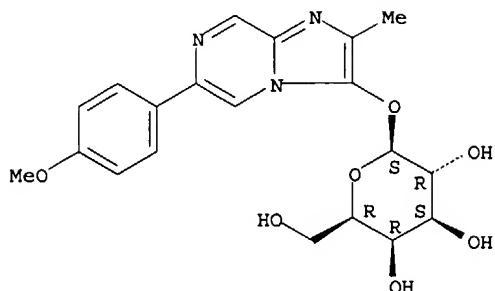
Absolute stereochemistry.



L28 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1995:992122 HCAPLUS
 DN 124:80192
 ED Entered STN: 20 Dec 1995
 TI Enhancement effect of 2,6-O-dimethyl-.beta.-cyclodextrin on the chemiluminescent detection of .beta.-D-galactosidase using a Cypridina luciferin analog
 AU Mitani, Motohiro; Sakaki, Syujiro; Koinuma, Yasumi; Toya, Yoshiaki; Kosugi, Masanori
 CS Tsukuba Res. Lab., NOF Corp., Tsukuba, 300-26, Japan
 SO Analytical Sciences (1995), 11(6), 1013-15
 CODEN: ANSCEN; ISSN: 0910-6340
 PB Japan Society for Analytical Chemistry
 DT Journal
 LA English
 CC 7-1 (Enzymes)
 Section cross-reference(s): 9
 AB .beta.-Cyclodextrins enhanced the chemiluminescent detection of .beta.-galactosidase using the Cypridina luciferin analog 3-(.beta.-Galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-*alpha*]pyrazine (.beta.-Gal-MCLA) in the order 2,6-O-dimethyl-.beta.-cyclodextrin > 2,3,6-O-trimethyl-.beta.-cyclodextrin > .beta.-cyclodextrin. Detection of mouse IgG by chemiluminescent enzyme immunoassay (CLEIA) using .beta.-Gal-MCLA and .beta.-galactosidase to amplify the signal was also enhanced by inclusion of 2,6-O-trimethyl-.beta.-cyclodextrin.
 ST galactosidase beta detn chemiluminescence beta cyclodextrin; IgG detn chemiluminescent enzyme immunoassay cyclodextrin
 IT Luminescence, chemi-
 (enhancement effect of 2,6-O-dimethyl-.beta.-cyclodextrin on the chemiluminescent detection of .beta.-D-galactosidase using a Cypridina luciferin analog)
 IT Immunoglobulins
 RL: ANT (Analyte); ANST (Analytical study)
 (G, ant; enhancement effect of 2,6-O-dimethyl-.beta.-cyclodextrin on the chemiluminescent detection of .beta.-D-galactosidase using a Cypridina luciferin analog)
 IT Immunoassay
 (chemiluminescence enzyme, enhancement effect of 2,6-O-dimethyl-.beta.-cyclodextrin on the chemiluminescent detection of .beta.-D-galactosidase using a Cypridina luciferin analog)
 IT 9031-11-2
 RL: ANT (Analyte); ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
 (enhancement effect of 2,6-O-dimethyl-.beta.-cyclodextrin on the chemiluminescent detection of .beta.-D-galactosidase using a Cypridina luciferin analog)
 IT 7585-39-9, .beta.-Cyclodextrin 51166-71-3, 2,6-O-Dimethyl-.beta.-cyclodextrin 55216-11-0, 2,3,6-O-Trimethyl-.beta.-cyclodextrin 159503-66-9
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
 (enhancement effect of 2,6-O-dimethyl-.beta.-cyclodextrin on the chemiluminescent detection of .beta.-D-galactosidase using a Cypridina luciferin analog)
 IT 159503-66-9
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
 (enhancement effect of 2,6-O-dimethyl-.beta.-cyclodextrin on the chemiluminescent detection of .beta.-D-galactosidase using a Cypridina luciferin analog)
 RN 159503-66-9 HCAPLUS
 CN .beta.-D-Galactopyranoside, 6-(4-methoxyphenyl)-2-methylimidazo[1,2-

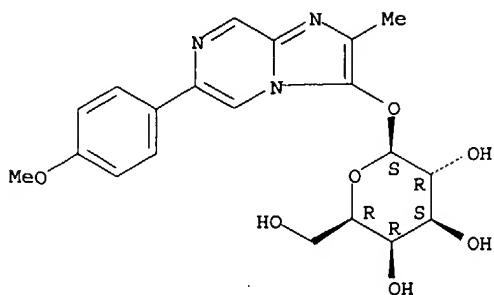
a]pyrazin-3-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.

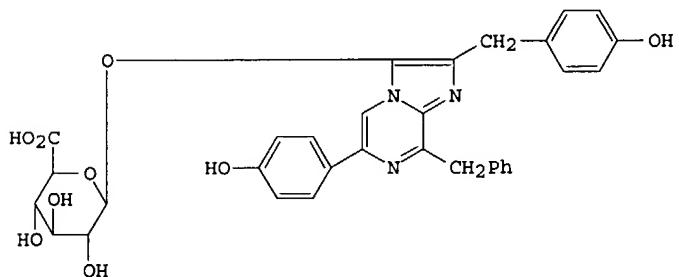


L28 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1995:126975 HCAPLUS
 DN 122:4783
 ED Entered STN: 08 Nov 1994
 TI Chemiluminescent assay of .beta.-D-galactosidase using Cypridina luciferin analog: 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazine
 AU Mitani, Motohiro; Sakaki, Syujiro; Koinuma, Yasumi; Toya, Yoshiaki; Kosugi, Masanori
 CS Tsukuba Res. Lab., NOF Corp., Ibaraki, 300-26, Japan
 SO Analytical Sciences (1994), 10(5), 813-14
 CODEN: ANSCEN; ISSN: 0910-6340
 DT Journal
 LA English
 CC 9-10 (Biochemical Methods)
 AB We prepared a new Cypridina luciferin analog, 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazine (.beta.-Gal-MCLA) which can enzymically remove galactose to produce 2-methyl-6-(4-methoxyphenyl)-3,7-dihydroimidazo[1,2-a]pyrazine-3(7H)-one (MCLA), its autoxidn. follows, providing the chemiluminescence. .beta.-Gal-MCLA was thus a useful chemiluminescent substrate for .beta.-D-Galactosidase determination
 ST galactosidase chemiluminescence galactopyranosyloxy methoxyphenyl methylimidazo pyrazine
 IT 9031-11-2, .beta.-D-Galactosidase
 RL: ANT (Analyte); ANST (Analytical study)
 (chemiluminescent assay of .beta.-D-galactosidase using Cypridina luciferin analog: 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazine)
 IT 159503-66-9
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
 (chemiluminescent assay of .beta.-D-galactosidase using Cypridina luciferin analog: 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazine)
 IT 144465-03-2
 RL: ARU (Analytical role, unclassified); ANST (Analytical study)
 (chemiluminescent assay of .beta.-D-galactosidase using Cypridina luciferin analog: 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazine)
 IT 118877-07-9
 RL: ARU (Analytical role, unclassified); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent)
 (chemiluminescent assay of .beta.-D-galactosidase using Cypridina luciferin analog: 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazine)
 IT 159503-66-9
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
 (chemiluminescent assay of .beta.-D-galactosidase using Cypridina luciferin analog: 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazine)
 RN 159503-66-9 HCAPLUS
 CN .beta.-D-Galactopyranoside, 6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazin-3-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



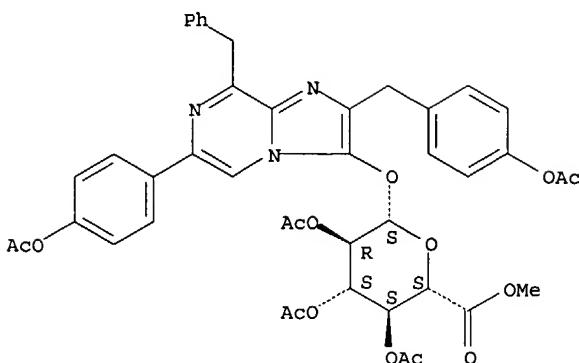
L28 ANSWER 6 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
 AN 1987:153383 HCPLUS
 DN 106:153383
 ED Entered STN: 15 May 1987
 TI Chemical studies of myctophina fish bioluminescence
 AU Inoue, Shoji; Okada, Kunisuke; Tanino, Hideo; Kakoi, Hisae
 CS Fac. Pharm., Meijo Univ., Nagoya, 468, Japan
 SO Chemistry Letters (1987), (2), 417-18
 CODEN: CMLTAG; ISSN: 0366-7022
 DT Journal
 LA English
 CC 12-1 (Nonmammalian Biochemistry)
 Section cross-reference(s): 26
 GI



I

AB A new type of masked watasenia preluciferin was isolated from the liver of a myctophina fish (*Diaphus elucens*) and its structure was determined as watasenia preluciferyl .beta.-D-glucopyranosiduronic acid (I).
 ST Diaphus liver watasenia preluciferyl glucopyranosidurate; myctophina fish watasenia preluciferyl glucopyranosidurate
 IT *Diaphus elucens*
 (watasenia preluciferyl glucopyranosidurate of liver of)
 IT Liver, composition
 (watasenia preluciferyl glucopyranosidurate of, of myctophina fish)
 IT 107503-11-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (deacetylation of)
 IT 65417-18-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (esterification of)
 IT 107503-09-3
 RL: BIOL (Biological study)
 (of liver, of myctophina fish)
 IT 55779-48-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 107503-11-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (deacetylation of)
 RN 107503-11-7 HCPLUS
 CN .beta.-D-Glucopyranosiduronic acid, 6-[4-(acetoxy)phenyl]-2-[[4-(acetoxy)phenyl]methyl]-8-(phenylmethyl)imidazo[1,2-a]pyrazin-3-yl (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



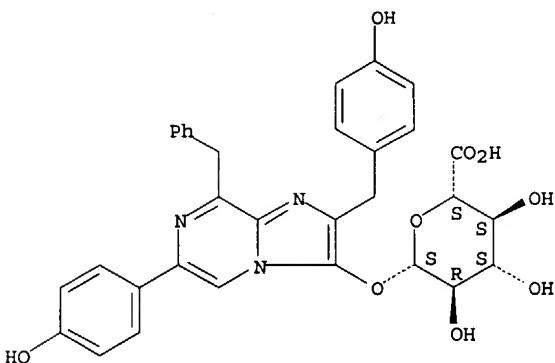
IT 107503-09-3

RL: BIOL (Biological study)
(of liver, of myctophina fish)

RN 107503-09-3 HCAPLUS

CN .beta.-D-Glucopyranosiduronic acid, 6-[(4-hydroxyphenyl)methyl]-8-(phenylmethyl)imidazo[1,2-a]pyrazin-3-yl (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1985:55384 HCAPLUS

DN 102:55384

ED Entered STN: 09 Feb 1985

TI Carbon-13 nuclear magnetic resonance spectra in the identification of N-, O- or S-methyl derivatives of some tautomeric hydroxy and mercapto nitrogen heterocycles

AU Barlin, Gordon B.; Brown, Desmond J.; Fenn, M. David

CS John Curtin Sch. Med. Res., Aust. Natl. Univ., Canberra, 2601, Australia

SO Australian Journal of Chemistry (1984), 37(11), 2391-5

CODEN: AJCHAS; ISSN: 0004-9425

DT Journal

LA English

CC 80-5 (Organic Analytical Chemistry)

Section cross-reference(s): 22

AB Carbon-13 NMR spectroscopy, in contrast to 1H NMR spectroscopy, has been shown to provide a clear distinction in a variety of N heterocyclic systems between O-Me and nuclear N-Me groups. MeO groups occur in the range δ . 53.20-61.87, nuclear N-Me groups at 34.29-49.62, and MeS groups at 12.35-14.55 for the compds. examined in CDCl_3 . Data for N- and O-Me derivs. of pyridin-2 and -4-ol, the corresponding pyrimidines, and some S analogs were compared with those for the unmethylated parent compds.

ST nitrogen heterocycle tautomer identification NMR; carbon 13 NMR tautomer identification

IT Tautomerism and Tautomers

(of Me derivs. of hydroxy and mercaptonitrogen heterocyclic compds.,

carbon-13 NMR identification of)

IT Spectrochemical analysis
(NMR, carbon-13, in identification of Me derivs. of tautomeric hydroxy and mercapto nitrogen heterocyclic compds.)

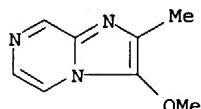
IT Heterocyclic compounds
RL: ANST (Analytical study)
(nitrogen, identification of Me derivs. of tautomeric hydroxy and mercapto, carbon-13 NMR spectrometric)

IT 83-54-5 142-08-5 557-01-7 620-08-6 626-64-2 694-85-9 695-19-2
823-09-6 931-63-5 1628-89-3 1722-10-7 2044-27-1 2228-30-0
2637-34-5 3739-81-9 4556-23-4 4562-27-0 6104-41-2 6104-45-6
6104-46-7 6887-59-8 18438-38-5 22581-72-2 53745-18-9 73547-86-1
79690-90-7 79690-93-0 87814-34-4 87814-37-7 87814-38-8
94317-79-0 94317-80-3
RL: ANST (Analytical study)
(identification of, carbon-13 NMR spectrometric)

IT 87814-38-8
RL: ANST (Analytical study)
(identification of, carbon-13 NMR spectrometric)

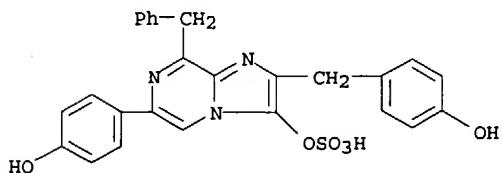
RN 87814-38-8 HCPLUS

CN Imidazo[1,2-al]pyrazine, 3-methoxy-2-methyl- (9CI) (CA INDEX NAME)



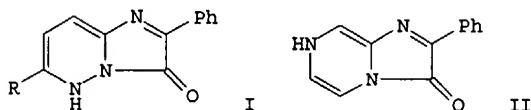
L28 ANSWER 8 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
AN 1984:468065 HCPLUS
DN 101:68065
ED Entered STN: 01 Sep 1984
TI Mechanism of photoinactivation and re-activation in the bioluminescence system of the ctenophore Mnemiopsis
AU Anctil, Michel; Shimomura, Osamu
CS Mar. Biol. Lab., Woods Hole, MA, 02543, USA
SO Biochemical Journal (1984), 221(1), 269-72
CODEN: BIJOAK; ISSN: 0306-3275
DT Journal
LA English
CC 6-3 (General Biochemistry)
Section cross-reference(s): 12
AB The bioluminescence of *M. leidyi* takes place when the photoprotein mnemiopsin in the photocytos reacts with Ca²⁺. The luminescence is inhibited in sunlight and this photoinhibition is reversible by keeping the live specimens in the dark. Exts. of mnemiopsin are similarly photoinhibited, but the photoinhibition cannot be reversed in the dark. Photoinhibited mnemiopsin can be reactivated in the dark by incubation with coelenterazine and O₂ only in solns. having a pH very close to 9.0. The reactivation in vivo probably takes place in the same manner, using the coelenterazine that is supplied from its abundant storage form. Apparently, photoinactivation of mnemiopsin results in the dissociation of coelenterazine and O₂ from the mol. of photoprotein; the dissociated form of the former mol. is an inactive form of coelenterazine, not free coelenterazine.
ST bioluminescence Mnemiopsis photoinactivation; mnemiopsin light inactivation coelenterazine oxygen; ctenophore bioluminescence photoinactivation; luminescence bio Mnemiopsis
IT Light, biological effects
(bioluminescence of ctenophore inactivation by, reactivation by coelenterazine and oxygen in relation to)
IT Mnemiopsis leidyi
(bioluminescence of, light inactivation of, reactivation by coelenterazine and oxygen in relation to)
IT Luminescence, bio-
(of ctenophore, light inactivation of, reactivation by coelenterazine and oxygen in relation to)
IT Proteins
RL: BIOL (Biological study)
(mnemiopsins, light inactivation of, reactivation by coelenterazine and oxygen in relation to)
IT 7782-44-7, biological studies
RL: BIOL (Biological study)

IT 55779-48-1
 RL: BIOL (Biological study)
 (mnemiopsin activation by oxygen and)
 IT 55779-48-1D, oxidized 65417-14-3
 RL: BIOL (Biological study)
 (of ctenophore)
 IT 65417-14-3
 RL: BIOL (Biological study)
 (of ctenophore)
 RN 65417-14-3 HCAPLUS
 CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)methyl]-, 3-(hydrogen sulfate), monosodium salt (9CI) (CA INDEX NAME)



● Na

L28 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1983:594926 HCAPLUS
 DN 99:194926
 ED Entered STN: 12 May 1984
 TI Imidazo[1,2-b]pyridazines and an imidazo[1,2-a]pyrazine from pyridazin- and pyrazinamines
 AU Barlin, Gordon B.; Brown, Desmond J.; Kadunc, Zdenka; Petric, Andrej; Stanovnik, Branka; Tisler, Miha
 CS John Curtin Sch. Med. Res., Canberra, 2601, Australia
 SO Australian Journal of Chemistry (1983), 36(6), 1215-20
 CODEN: AJCHAS; ISSN: 0004-9425
 DT Journal
 LA English
 CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
 OS CASREACT 99:194926
 GI



AB The ambiguous condensations of PhCOCHO with pyridazin-3-amines and pyrazin-2-amine give imidazopyridazinones I (R = H, Cl) and imidazopyrazinone II; resp. The former products exist as such, at least in the solid state, whereas the latter product exists to a large extent as the corresponding dipolar mol. The reactions, degrdns., and NMR spectra of the products are discussed.
 ST imidazopyrazine; imidazopyridazine; phenylglyoxal cyclization
 pyridazinamine pyrazinamine
 IT 6342-56-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclization of, with chloropyridinamine, imidazopyrazidine derivative)
 IT 5469-69-2 5469-70-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclization of, with phenylglyoxal, imidazopyrazinone derivative from)
 IT 5049-61-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclization of, with phenylglyoxal, phenylimidazolpyrazinone from)
 IT 1074-12-0
 RL: RCT (Reactant); RACT (Reactant or reagent)

(cyclization of, with pyridazinamines and pyrazinamines,
imidazolpyrazinone and imidazopyrazinone derivs. from)

IT 87814-32-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and methylation of)

IT 87814-31-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reactions of)

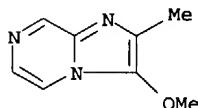
IT 27955-58-4P 87814-33-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and ring cleavage of)

IT 87814-34-4P 87814-35-5P 87814-36-6P 87814-37-7P 87814-38-8P
87814-39-9P 87814-40-2P 87814-41-3P 87814-42-4P 87814-43-5P
87814-44-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 87814-38-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

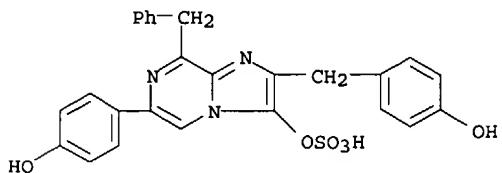
RN 87814-38-8 HCPLUS

CN Imidazo[1,2-a]pyrazine, 3-methoxy-2-methyl- (9CI) (CA INDEX NAME)



L28 ANSWER 10 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
AN 1980:107639 HCPLUS
DN 92:107639
ED Entered STN: 12 May 1984
TI Comparison of the amounts of key components in the bioluminescence systems
of various coelenterates
AU Shimomura, Osamu; Johnson, Frank H.
CS Dep. Biol., Princeton Univ., Princeton, NJ, 08540, USA
SO Comparative Biochemistry and Physiology, Part B: Biochemistry & Molecular
Biology (1979), 64B(1), 105-7
CODEN: CBPBB8; ISSN: 0305-0491
DT Journal
LA English
CC 12-1 (Nonmammalian Biochemistry)
AB Luciferase, photoprotein, free and protein-bound coelenterazine (I) and I
enol-sulfate were assayed and compared in 5 bioluminescent coelenterates.
Hydrozoans Aequorea aequorea and Halistaura cellularia contained
photoprotein plus very small amts. of I enol-sulfate and luciferase
activity, but no free I. Anthozoans Ptilosarcus gurneyi, Cavernularia
obesa, and Renilla muelleri contained luciferase, I, and I enol-sulfate,
but very little or no photoprotein. I existed mainly in a stabilized form
bound to a Ca-binding protein. The bioluminescent reactions in the
coelenterates were compared.
ST bioluminescence coelenterate; luciferase coelenterate bioluminescence;
coelenterazine coelenterate bioluminescence; photoprotein coelenterate
bioluminescence
IT Aequorea aequorea
Cavernularia obesa
Coelenterate
Halistaura cellularia
Ptilosarcus gurneyi
Renilla muelleri
(bioluminescence system components of)
IT Luminescence, bio-
(in coelenterates)
IT Proteins
RL: BIOL (Biological study)
(photo-, of coelenterates, bioluminescence in relation to)
IT 9014-00-0 55779-47-0 55779-48-1
RL: BIOL (Biological study)
(of coelenterates, bioluminescence in relation to)
IT 55779-47-0

RL: BIOL (Biological study)
 (of coelenterates, bioluminescence in relation to)
 RN 55779-47-0 HCPLUS
 CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)methyl]-8-(phenylmethyl)-, 3-(hydrogen sulfate) (9CI) (CA INDEX NAME)



L28 ANSWER 11 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
 AN 1979:519858 HCPLUS
 DN 91:119858
 ED Entered STN: 12 May 1984
 TI A Bioluminescence assay for PAP (3',5'-diphosphoadenosine) and PAPS (3'-phosphoadenylyl sulfate)
 AU Anderson, James Michael; Hori, Kazuo; Cormier, Milton J.
 CS Boyd Grad. Stud. Res. Cent., Univ. Georgia, Athens, GA, 30602, USA
 SO Methods in Enzymology (1978), 57(Biolumin. Chemilumin.), 244-57
 CODEN: MENZAU; ISSN: 0076-6879
 DT Journal
 LA English
 CC 9-6 (Biochemical Methods)
 AB Procedures in the bioluminescence assay of PAP and PAPS using the luciferin-luciferase reaction in *Renilla reniformis* are described. The assay is sensitive to 0.1 pmol of PAP. The synthesis of the substrate benzyl luciferyl sulfate and isolation of luciferin sulfokinase and luciferase are also described.
 ST diphosphoadenosine detn bioluminescence assay; PAPS detn bioluminescence
 IT Spinach
 (diphosphoadenosine and PAPS determination in leaves of, bioluminescence assay for)
 IT Heart, composition
 Kidney, composition
 Liver, composition
 Lung, composition
Photobacterium fischeri
 (diphosphoadenosine and PAPS determination in, bioluminescence assay for)
 IT Potato
 (diphosphoadenosine and PAPS determination in tubers of, bioluminescence assay for)
 IT *Renilla reniformis*
 (luciferase and luciferin sulfokinase isolation from, for diphosphoadenosine and PAPS bioluminescence assay)
 IT 71369-26-1
 RL: ANST (Analytical study)
 (condensation of, with aminobenzylmethoxyphenylpyrazine Me ether)
 IT 40040-81-1
 RL: ANST (Analytical study)
 (condensation of, with benzyl glyoxal di-Et acetal)
 IT 482-67-7 1053-73-2
 RL: ANT (Analyte); ANST (Analytical study)
 (determination of, bioluminescence assay for)
 IT 9014-00-0 37278-33-4
 RL: PROC (Process)
 (isolation of, of *Renilla reniformis* for diphosphoadenosine and PAPS bioluminescence assay)
 IT 50909-83-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and demethylation of)
 IT 71369-28-3P
 RL: PREP (Preparation)
 (preparation of, as substrate for diphosphoadenosine and PAPS bioluminescence assay)
 IT 71369-27-2
 RL: RCT (Reactant); RACT (Reactant or reagent)

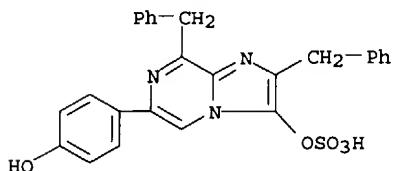
IT 9016-17-5
 (reaction of, with aryl sulfatase)
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with benzyl luciferyl disulfate)

IT 50909-86-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (sulfonation of)

IT 71369-28-3P
 RL: PREP (Preparation)
 (preparation of, as substrate for diphosphoadenosine and PAPS
 bioluminescence assay)

RN 71369-28-3 HCPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2,8-bis(phenylmethyl)-,
 3-(hydrogen sulfate), monopotassium salt (9CI) (CA INDEX NAME)

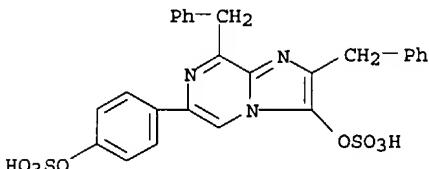


● K

IT 71369-27-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with aryl sulfatase)

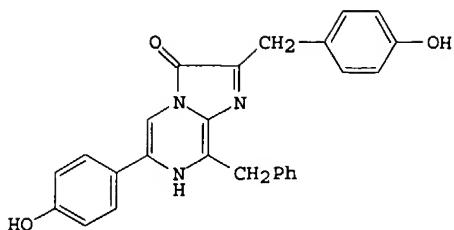
RN 71369-27-2 HCPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 2,8-bis(phenylmethyl)-6-[4-(sulfoxy)phenyl]-,
 hydrogen sulfate (ester), dipotassium salt (9CI) (CA INDEX NAME)

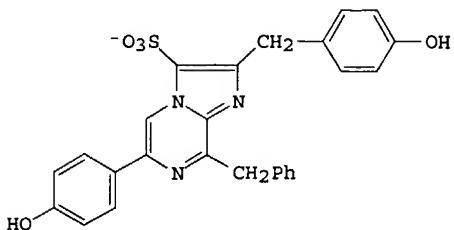


● 2 K

L28 ANSWER 12 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
 AN 1978:50764 HCPLUS
 DN 88:50764
 ED Entered STN: 12 May 1984
 TI Complete structure of Renilla luciferin and luciferyl sulfate
 AU Inoue, Shoji; Kakoi, Hisae; Murata, Mikiko; Goto, Toshio; Shimomura, Osamu
 CS Fac. Pharm., Meijo Univ., Nagoya, Japan
 SO Tetrahedron Letters (1977), (31), 2685-8
 CODEN: TELEAY; ISSN: 0040-4039
 DT Journal
 LA English
 CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
 GI



I



II

AB Examination of *Renilla* exts. showed that *Renilla luciferin* is coelenterazine (I). The structure of natural luciferyl sulfate was determined as II by comparison of natural and synthetic II. II was synthesized from I by sequential treatment with (AcO)2O, MeOH/NH3, and pyridine-SO3 complex and hydrolysis with MeOH/NaOH.

ST *Renilla luciferin* structure; luciferyl sulfate *Renilla* prep

IT 65417-16-5P 65417-17-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

IT 65417-14-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and structure of)

IT 65417-18-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and sulfonation of)

IT 61369-28-6P 65417-15-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 55779-48-1

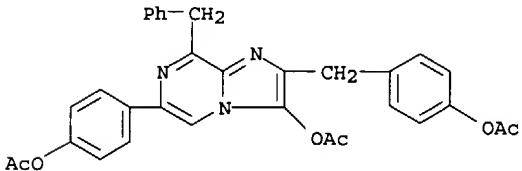
RL: RCT (Reactant); RACT (Reactant or reagent)
(structure, sulfonylation, and acetylation of)

IT 65417-16-5P 65417-17-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

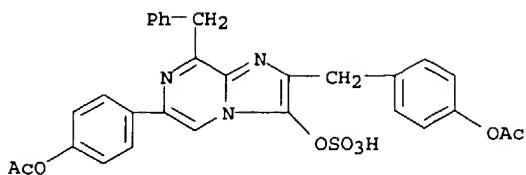
RN 65417-16-5 HCAPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 6-[4-(acetoxy)phenyl]-2-[[4-(acetoxy)phenyl]methyl]-8-(phenylmethyl)-, acetate (ester) (9CI) (CA INDEX NAME)



RN 65417-17-6 HCAPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 6-[4-(acetoxy)phenyl]-2-[[4-(acetoxy)phenyl]methyl]-8-(phenylmethyl)-, hydrogen sulfate (ester), sodium salt (9CI) (CA INDEX NAME)

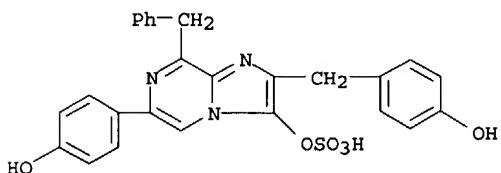


● Na

IT 65417-14-3P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and structure of)

RN 65417-14-3 HCPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)methyl]-, 3-(hydrogen sulfate), monosodium salt (9CI) (CA INDEX NAME)

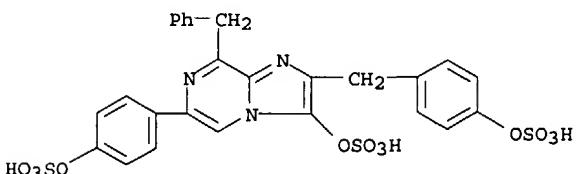


● Na

IT 65417-15-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 65417-15-4 HCPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 8-(phenylmethyl)-6-[4-(sulfooxy)phenyl]-2-[(4-(sulfooxy)phenyl)methyl]-, hydrogen sulfate (ester), trisodium salt (9CI) (CA INDEX NAME)



● 3 Na

L28 ANSWER 13 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN

AN 1977:596264 HCPLUS

DN 87:196264

ED Entered STN: 12 May 1984

TI Substrate and substrate analog binding properties of Renilla luciferase

AU Matthews, John C.; Hori, Kazuo; Cormier, Milton J.

CS Dep. Biochem., Univ. Georgia, Athens, GA, USA

SO Biochemistry (1977), 16(24), 5217-20

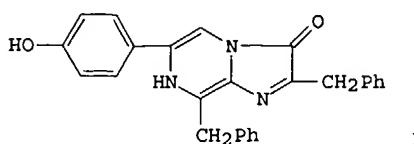
CODEN: BICHAW; ISSN: 0006-2960

DT Journal

LA English

CC 7-3 (Enzymes)

GI



AB The binding characteristics of luciferin, luciferin analogs (e.g. I), and competitive inhibitors of the luciferin-luciferase reaction were studied. Luciferin binding and orientation in the single luciferin binding site of luciferase from *R. reniformis* are highly specific for and dependent upon the 3 group substituents of the luciferin mol., whereas the imidazolone-pyrazine nucleus of luciferin is not directly involved in binding. Anaerobic luciferin binding promotes a rapid concentration-dependent aggregation of luciferase which results in irreversible inactivation of the enzyme. This aggregation phenomenon is not observed upon binding of oxyluciferin, luciferyl sulfate, or luciferin analogs in which the substituent at the 2 position of the imidazolone-pyrazine ring has been substantially altered.

ST luciferase substrate analog binding; *Renilla* luciferase substrate binding

IT *Renilla reniformis*

(luciferase of, inhibitor and substrate binding by)

IT Kinetics, enzymic

(of inhibition, of luciferase)

IT 51-67-2 100-46-9, reactions 103-49-1 104-94-9 108-88-3, reactions 108-95-2, reactions 6373-46-2 17297-75-5 19943-97-6 37156-84-6 40040-83-3 50909-85-8 50909-86-9 55779-47-0 55779-48-1 64750-82-9 64750-83-0 64750-84-1

RL: PROC (Process)

(luciferase binding of, structural factors in)

IT 9014-00-0

RL: BIOL (Biological study)

(of *Renilla*, inhibitor and substrate binding by, structural factors in)

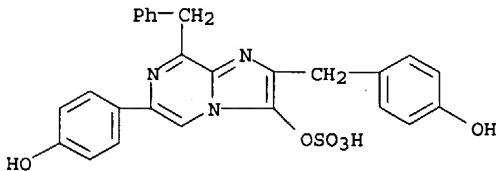
IT 55779-47-0 64750-83-0

RL: PROC (Process)

(luciferase binding of, structural factors in)

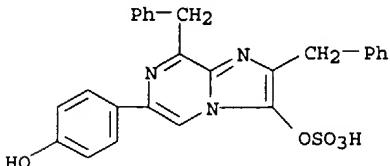
RN 55779-47-0 HCPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)methyl]-8-(phenylmethyl)-, 3-(hydrogen sulfate) (9CI) (CA INDEX NAME)



RN 64750-83-0 HCPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2,8-bis(phenylmethyl)-, 3-(hydrogen sulfate) (9CI) (CA INDEX NAME)



L28 ANSWER 14 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN

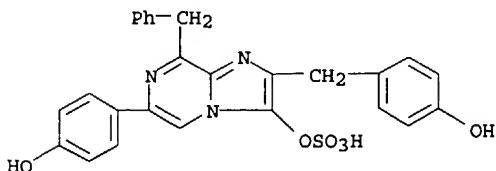
AN 1975:405600 HCPLUS

DN 83:5600

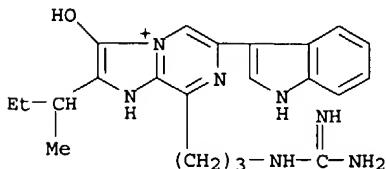
ED Entered STN: 12 May 1984

TI Chemical nature of bioluminescence systems in coelenterates

AU Shimomura, Osamu; Johnson, Frank H.
 CS Dep. Biol., Princeton Univ., Princeton, NJ, USA
 SO Proceedings of the National Academy of Sciences of the United States of America (1975), 72(4), 1546-9
 CODEN: PNASA6; ISSN: 0027-8424
 DT Journal
 LA English
 CC 12-13 (Nonmammalian Biochemistry)
 AB Anal. of substances involved in light-emitting reactions among bioluminescent coelenterates revealed a pronounced uniformity in the structural features of initial reactants, i.e., luciferins and photoprotein chromophores, as well as the light-emitter product. This product is structurally identical among the different classes of coelenterates; i.e., Hydrozoa (the jellyfish, Aequorea), Anthozoa (the sea cactus, Cavernularia; sea pansy, Renilla; and sea pen, Leioptilus), and very likely also the Scyphozoa (the jellyfish, Pelagia). In each of these instances the reaction product, 2-(p-hydroxyphenylacetyl)amino-3-benzyl-5-(p-hydroxyphenyl) pyrazine, is the actual light-emitter, whether it occurs in a Ca^{2+} -triggered photoprotein type of luminescence or in a luciferin-luciferase type. The evidence indicates that in certain coelenterates, e.g., Cavernularia, these 2 types are equally significant, whereas in others (Renilla and Leioptilus) the luciferin-luciferase type predominates over the Ca -triggerable photoprotein type. Only the photoprotein type functions in the luciferaseless jellyfish, Aequorea. In all instances investigated, the structure of the light-emitter prior to the luminescence reaction appears to be essentially the same as that of the chromophore of unreacted aequorin. The product of the luminescence reaction is absent in exts. of nonluminous species. However, a product very similar to that of luminescent coelenterates occurs also in representatives of other phyla, including the cephalopod molluscs, e.g., the "firefly squid" Watasenia and probably various ctenophores as well.
 ST bioluminescence coelenterate hydroxyphenylacetylaminobenzylhydroxyphenyl pyrazine; pyrazine deriv bioluminescence coelenterate
 IT Luminescence
 (bio-, of coelenterates, (hydroxyphenylacetyl)aminobenzyl(hydroxyphenyl) pyrazine in)
 IT Aequorea aequorea
 Cavernularia obesa
 Coelenterate
 Leioptilus
 Leptogorgia virgulata
 Renilla
 (bioluminescence of, (hydroxyphenylacetyl)aminobenzyl(hydroxyphenyl) pyrazine in)
 IT Nomenclature, new natural products
 (coelenteramide)
 IT Nomenclature, new natural products
 (coelenterazine)
 IT Luciferins
 RL: BIOL (Biological study)
 (sulfate, of bioluminescence species, product of)
 IT 50611-86-4 55779-48-1
 RL: BIOL (Biological study)
 (in bioluminescence, in coelenterates)
 IT 37156-84-6 55779-47-0
 RL: BIOL (Biological study)
 (in calcium-induced luminescence of coelenterates)
 IT 55779-47-0
 RL: BIOL (Biological study)
 (in calcium-induced luminescence of coelenterates)
 RN 55779-47-0 HCAPLUS
 CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)methyl]-8-(phenylmethyl)-, 3-(hydrogen sulfate) (9CI) (CA INDEX NAME)



L28 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1973:145460 HCAPLUS
 DN 78:145460
 ED Entered STN: 12 May 1984
 TI Exchange of oxygen between solvent water and the carbon dioxide produced in Cypridina bioluminescence
 AU Shimomura, Osamu; Johnson, Frank H.
 CS Biol. Dep., Princeton Univ., Princeton, NJ, USA
 SO Biochemical and Biophysical Research Communications (1973), 51(3), 558-63
 CODEN: BBRCA9; ISSN: 0006-291X
 DT Journal
 LA English
 CC 12-2 (Nonmammalian Biochemistry)
 AB Bioluminescent oxidation of Cypridina luciferin yields CO₂ besides oxyluciferin and light. The exchange of O between the CO₂ and H₂O of the solvent becomes significant when <1.μ.mole of luciferin is reacted in 4 ml of buffer solution, and the exchange O in CO₂ markedly increases by decreasing the amount of luciferin. Such an exchange is to be expected in any such system which produces CO₂ in aqueous solution, and must be taken into account in interpreting the results of expts.
 ST luciferin oxidn bioluminescence; Cypridina bioluminescence
 IT Luminescence
 (bio-, luciferin oxidation in)
 IT Cypridina
 (luminescence of, oxygen exchange between carbon dioxide and water in)
 IT Exchange reaction
 (of oxygen, between carbon dioxide and water in Cypridina bioluminescence)
 IT 7782-44-7, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (exchange reaction of, between carbon dioxide and water in Cypridina bioluminescence)
 IT 7732-18-5
 RL: BIOL (Biological study)
 (exchange reactions of oxygen in, with carbon dioxide, in Cypridina bioluminescence)
 IT 124-38-9, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (exchange reactions of oxygen in, with water, in Cypridina bioluminescence)
 IT 26008-71-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of, in bioluminescence)
 IT 26008-71-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of, in bioluminescence)
 RN 26008-71-9 HCAPLUS
 CN 1H-Imidazo[1,2-a]pyrazin-4-ium, 8-[3-[(aminoiminomethyl)amino]propyl]-3-hydroxy-6-(1H-indol-3-yl)-2-(1-methylpropyl)-, bromide, monohydrobromide (9CI) (CA INDEX NAME)

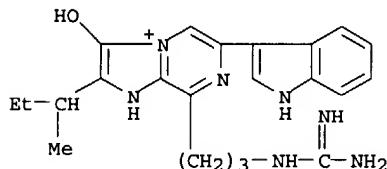


● Br⁻

● HBr

L28 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1970:432730 HCAPLUS

DN 73:32730
 ED Entered STN: 12 May 1984
 TI Chemistry of bioluminescence
 AU Goto, Toshio
 CS Dep. Agr. Chem., Nagoya Univ., Nagoya, Japan
 SO Pure and Applied Chemistry (1968), 17(3-4), 421-41
 CODEN: PACHAS; ISSN: 0033-4545
 DT Journal; General Review
 LA English
 CC 9 (Nonmammalian Biochemistry)
 AB The bioluminescence kinetics and mechanisms of *Cypridina hilgendorfii* luciferin and related compds. is reviewed. 40 refs.
 ST Cypridina bioluminescence review; bioluminescence kinetics; kinetics bioluminescence; luciferin luciferase kinetics; review bioluminescence luciferin
 IT Luminescence
 (bio-, of *Cypridina hilgendorfii*)
 IT *Cypridina*
 (hilgendorfii, bioluminescence of)
 IT 26008-71-9
 RL: PRP (Properties)
 (bioluminescence of, of *Cypridina hilgendorfii*)
 IT 26008-71-9
 RL: PRP (Properties)
 (bioluminescence of, of *Cypridina hilgendorfii*)
 RN 26008-71-9 HCPLUS
 CN 1H-Imidazo[1,2-a]pyrazin-4-ium, 8-[3-[(aminoiminomethyl)amino]propyl]-3-hydroxy-6-(1H-indol-3-yl)-2-(1-methylpropyl)-, bromide, monohydrobromide (9CI) (CA INDEX NAME)

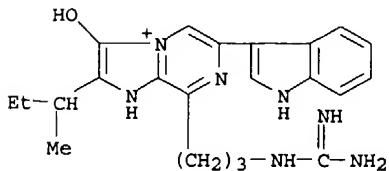


● Br⁻

● HBr

L28 ANSWER 17 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
 AN 1970:107330 HCPLUS
 DN 72:107330
 ED Entered STN: 12 May 1984
 TI Enzyme catalyzed oxidation of *Cypridina luciferin*
 AU Stone, Henry
 CS Princeton Univ., Princeton, NJ, USA
 SO (1969) 80 pp. Avail.: 69-14,438
 From: Diss. Abstr. Int. B 1969, 30(3), 1020-1
 DT Dissertation
 LA English
 CC 3 (Enzymes)
 AB Unavailable
 ST *Cypridina luciferin* oxidn; luciferin enzymic oxidn
 IT Enzymes
 RL: BIOL (Biological study)
 (luciferin-oxidizing, of *Cypridina*)
 IT 26008-71-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of, enzymic)
 IT 26008-71-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (oxidation of, enzymic)
 RN 26008-71-9 HCPLUS
 CN 1H-Imidazo[1,2-a]pyrazin-4-ium, 8-[3-[(aminoiminomethyl)amino]propyl]-3-

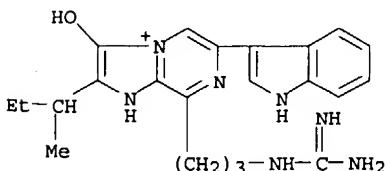
hydroxy-6-(1H-indol-3-yl)-2-(1-methylpropyl)-, bromide, monohydrobromide
(9CI) (CA INDEX NAME)



● Br⁻

● HBr

L28 ANSWER 18 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
 AN 1970:62631 HCPLUS
 DN 72:62631
 ED Entered STN: 12 May 1984
 TI Bioluminescence and mechanism of luminescence
 AU Got, Toshio
 CS Nagoya Univ., Nagoya, Japan
 SO Kagaku to Seibutsu (1969), 7(8), 445-51
 CODEN: KASEAA; ISSN: 0453-073X
 DT Journal; General Review
 LA Japanese
 CC 2 (General Biochemistry)
 AB A review. Mechanism of chemiluminescence was outlined with special reference to the formation of an intermediate hydroperoxide anion and its decomposition through 4-membered ring peroxide into carbonyl compound in singlet excited state, and illustrated by Cypridina luciferin. 28 refs.
 ST bioluminescence review; review bioluminescence; luminescence review
 IT Luminescence
 (bio-, mechanism of)
 IT 26008-71-9
 RL: PRP (Properties)
 (luminescence of, mechanism of)
 IT 26008-71-9
 RL: PRP (Properties)
 (luminescence of, mechanism of)
 RN 26008-71-9 HCPLUS
 CN 1H-Imidazo[1,2-a]pyrazin-4-ium, 8-[3-[(aminoiminomethyl)amino]propyl]-3-hydroxy-6-(1H-indol-3-yl)-2-(1-methylpropyl)-, bromide, monohydrobromide
(9CI) (CA INDEX NAME)

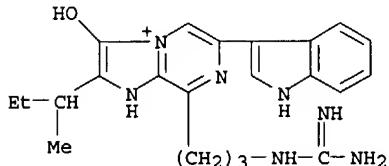


● Br⁻

● HBr

L28 ANSWER 19 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN

AN 1968:46251 HCPLUS
 DN 68:46251
 ED Entered STN: 12 May 1984
 TI Bioluminescence. Cypridina luciferin
 AU Hirata, Yoshimasa; Goto, Toshio
 CS Nagoya Univ., Nagoya, Japan
 SO Kagaku (Tokyo, Japan) (1967), 37(12), 640-6
 CODEN: KAGTAT; ISSN: 0022-7625
 DT Journal
 LA Japanese
 CC 2 (General Biochemistry)
 GI For diagram(s), see printed CA Issue.
 AB The scheme of bioluminescence reaction of luciferin can be represented: luciferin + O₂ - (luciferase).fwdarw. oxyluciferin +hv. Oxyluciferin was gradually decomposed to etioluciferin (I). From further studies on the structure of luciferin, the new structure II was proposed. Attempts to synthesize II gave a very poor yield.
 ST BIOLUMINESCENCE LUCIFERIN; ETIOLUCIFERIN; LUCIFERIN STRUCTURE ACTION; LUMINESCENCE LUCIFERIN
 IT Luminescence
 (bio-, of luciferin, intermediates in)
 IT Cypridina
 (luciferin of, bioluminescence of, intermediates in)
 IT Molecular structure
 (of luciferin)
 IT 19321-05-2
 RL: BIOL (Biological study)
 (luciferin (cypridina) identity with)
 IT 19321-05-2
 RL: BIOL (Biological study)
 (luciferin (cypridina) identity with)
 RN 19321-05-2 HCPLUS
 CN 1H-Imidazo[1,2-a]pyrazin-4-ium, 2-sec-butyl-8-(3-guanidinopropyl)-3-hydroxy-6-indol-3-yl-, bromide, monohydrobromide (8CI) (CA INDEX NAME)



● Br⁻

● HBr

L28 ANSWER 20 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
 AN 1967:432674 HCPLUS
 DN 67:32674
 ED Entered STN: 12 May 1984
 TI Structure of Cypridina luciferin
 AU Kishi, Yoshito; Goto, Toshio; Hirata, Yoshimasa; Shimomura, Osamu; Johnson, Frank Harris
 CS Fac. Sci., Nagoya Univ., Nagoya, Japan
 SO Biolumin. Prog., Proc. Conf. (1966), Meeting Date 1965, 89-113
 CODEN: 16HSAG
 DT Conference
 LA English
 CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
 GI For diagram(s), see printed CA Issue.
 AB Luciferin yields oxyluciferin (I) and etioluciferin (II) when treated with luciferase-O or NH₃-O. The former can be converted to the latter by acid treatment. Treatment of II with Ba(OH)₂ gives etioluciferamine. N.M.R. spectra and high-resolution mass spectra as well as chemical data confirm the structures of these compds. On the basis of structure II, the structure I can be assigned to oxyluciferin. The structure III is assigned to

luciferin hydrobromide and IV to luciferin hydrochloride. These structures comprise tryptamine, arginine, and isoleucine moieties.

ST STRUCTURE CYPRIDINA LUCIFERIN; LUCIFERIN CYPRIDINA STRUCTURE; ARGININE; ISOLEUCINE; ETIOLUCIFERIN; CYPRIDINA LUCIFERIN STRUCTURE

IT Cypridina
(luciferin of, structure of)

IT 1H-Imidazo[1,2-a]pyrazin-4-ium, 2-sec-butyl-8-(3-guanidinopropyl)-3-hydroxy-6-indol-3-yl-, hydroxide
Guanidine, [3-(2-sec-butyl-3,7-dihydro-6-indol-3-yl-3-oxoimidazo[1,2-a]pyrazin-8-yl)propyl]-
RL: RCT (Reactant); RACT (Reactant or reagent)
(as structure of luciferin)

IT Luciferin
Luciferin, bromide, hydrobromide
Luciferin, hydroxide
RL: PRP (Properties)
(structure of)

IT 7256-95-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(as structure of etioluciferamine)

IT 7269-75-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(as structure of etioluciferin)

IT 19321-05-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(as structure of luciferin hydrobromide)

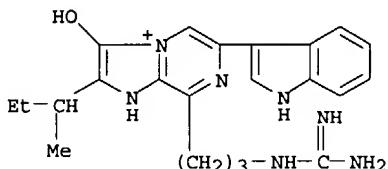
IT 10104-19-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(as structure of oxyluciferin)

IT 7256-95-3 7269-75-2 17297-78-8
RL: PRP (Properties)
(structure of)

IT 19321-05-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(as structure of luciferin hydrobromide)

RN 19321-05-2 HCPLUS

CN 1H-Imidazo[1,2-a]pyrazin-4-ium, 2-sec-butyl-8-(3-guanidinopropyl)-3-hydroxy-6-indol-3-yl-, bromide, monohydrobromide (8CI) (CA INDEX NAME)



● Br⁻

● HBr

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